DEPARTMENT OF COMMERCE ★ NATIONAL BUREAU OF STANDARDS ★

NBS MONOGRAPH 25—SECTION 17

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Standard X-ray Diffraction Powder Patterns

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Standard X-ray Diffraction Powder Patterns
Section 17—Data for 54 Substances

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STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Previous work has been published as a book entitled Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976) (JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081). The volume is sold with an accompanying search manual, and contains 949 card images of patterns of experimental data, published originally as Circular 539 (vols. 1-10) and Monograph 25, Sections 1-12, and most of Section 13.

Individual copies of the Circular and Monograph are still available and may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. If a publication listed below is identified with a number, it must be used in ordering. All are available in hardcopy or microfiche; the price is not fixed and will be furnished on request.

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	Volume 7	PB 178 908
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ERRATA

Monograph 25

Section 16, pp. iii, 66, 176, 183: The corrected formula for sodium borate hydroxide hydrate (borax) is $Na_2B_4O_5(OH)_4 \cdot 8H_2O$.

p. 1: In the 2nd column, last paragraph, line 5 from the bottom, the symbols should be $K\alpha_1$.

p. 129: In the paragraph "Structure", the space group should be $P2_1/c$.

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 17. --- Data for 54 Substances

by

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Standard x-ray diffraction patterns are presented for 54 substances. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured in some cases.

Key words: Crystal structure; lattice constants; powder patterns; reference intensities; standard; x-ray diffraction.

INTRODUCTION

The Powder Diffraction File is a continuing compilation of diffraction patterns gathered from many sources. Produced and published by the JCPDS--International Centre for Diffraction Data,[1] the File is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, the program at the National Bureau of Standards contributes new data to this File. Our work also aids in the evaluation and revision of published x-ray data and in the development of diffraction techniques. This report presents information for 54 experimental patterns, and is the twenty-seventh of the series of <u>Standard X-ray Diffraction Powder Patterns</u>.[2]

EXPERIMENTAL POWDER PATTERNS

<u>CAS registry number</u>. The Chemical Abstracts Service Registry Number is included, when available, to help identify the sample. This number forms the basis for computer aided searching of Chemical Abstracts.

<u>Sample</u>. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the samples improved the quality of most of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

<u>Optical data</u>. When reported, optical measurements were made by grain immersion methods, in white light, using oils standardized in sodium light, in the refractive index range 1.49 to 2.1 [Hartshorne and Stuart, 1970].

The names of the sample colors were selected from the ISCC-NBS Centroid Color Charts [1965].

<u>Interplanar spacings</u>. For spacing determinations, a shallow holder was packed with a sample mixed with an internal standard. Choice of the standard was determined by the need for low angle and unobstructed reflections. The amount of standard was estimated so that the intensity of its strongest peak would be about equal to the intensity of the strongest peak of the sample.

To avoid errors associated with aberrations at the very top of the peaks, the readings of 2θ were taken at positions about 20% of the way down from the top, and in the center of the peak width. The $K\alpha_2$ peaks were occasionally read to assist in establishing a $K\alpha_1$ peak position, but $K\alpha_2$ peaks were not reported.

At low angles, $K\alpha_1$ and $K\alpha_2$ peaks were unresolved for both the sample and the internal standard. The internal standard corrections were established from the theoretical values for $K\alpha_1$ and were applied to the unresolved low angle peaks, as well as to the resolved $K\alpha_1$ peaks in the higher angle regions. If the internal standard correction varied along th length of the pattern, linear interpolations were used.

[1]JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081. This Pennsylvania non-profit corporation functions in cooperation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, The Clay Minerals Society, The Institute of Physics, the Mineralogical Association of Canada, the Mineralogial Society of America, The Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Francaise de Minéralogie et de Cristallographie.

[2]See previous page for other published volumes.

The internal standards used were of high purity (99.99%). The lattice constants used for them at 25 °C are given in Table 1; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Table 1

Calculated 2θ Angles, CuKα_1 λ = 1.540598Å

hkℓ	W a=3.16524Å ±.00004	Ag a=4.08651Å ±.00002	Si a=5.43088Å ±.00004
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.303
310	100.632		
311		77.390	56.123
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.131
331		110.499	76.377
420		114.914	
422		134.871	88.032
511/333		156.737	94.954
440			106.710
531			114.094
620			127.547
533			136.897
444			158.638

The internal standard Si powder is available as Standard Reference Material 640 [1974]. The lattice constant for the Si was refined from multiple powder data measurements made with tungsten as an internal standard [Swanson et al., 1966]. Single crystal cell parameter data were also collected. The lattice parameters from the two methods agreed within three parts in 10^5 [Hubbard et al., 1975]. D-spacing results using SRM 640 will be in agreement with patterns recorded in this series of monographs since 1966.

All of our spacing measurements were recorded at 25 ± 1 °C on a diffractometer equipped with a focusing graphite or lithium fluoride crystal monochromator located between the sample and the scintillation counter. Pulse height discrimination was used as well. All measurements were performed using copper radiation: λ(CuKα_1, peak) = 1.540598Å [Deslattes and Henins, 1973].

Structure, lattice constants. The space groups were listed with short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography, Vol. I [1952].

Orthorhombic cell dimensions were arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants were transformed if necessary in order to follow the convention of Crystal Data [1973].

A computer program [Evans et al., 1963] assigned hkℓs and refined the lattice constants. Cell refinement was based only upon $2\theta_{obs}$ values which could be indexed without ambiguity. The program minimized the value $\Sigma(\theta_{obs}-\theta_{calc})^2$. The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants in earlier publications of this series. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

In indexing cubic patterns, for a given reflection multiple hkℓ's were not utilized in the refinement or reported. Instead, the single appropriate index having the largest h was listed. The number of significant figures reported for d-values varied with the symmetry and crystallinity of each sample.

The number of significant figures at any reported d-value was derived from the average error in $|2\theta_{obs} - 2\theta_{calc}|$ and $\Delta d/d = -\cot\theta\, \Delta\theta$. With these conditions, the rounding of any specific d at the given number of significant digits yielded an error in its corresponding 2θ which was less than the average error in 2θ.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943 x 10^{23} [Deslattes et al., 1974] and 1977 atomic weights published by the International Union of Pure and Applied Chemistry [1979].

Figure of merit. Several figures of merit ratings are available for assessing indexed powder data. M_{20} [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing. A value of $M_{20} > 10$ will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines ($X_{20} \leq 2$) [de Wolff, 1968]. In general, patterns reported in this publication had $M_{20} > 20$ and X = 0. M_{20} was specified for any pattern indexed with a cell derived only through computer indexing from powder data, without further confirmation.

The accuracy and completeness of measured interplanar spacings was conveniently reported as F_N [Smith and Snyder, 1979]. The format used in this publication was F_N = overall value ($\overline{|\Delta 2\theta|}$, N_{poss}), where N, the number of observed reflections was chosen as 30, or the maximum number of lines of the pattern if the entire pattern had fewer than 30 lines. The "overall value" was the figure of merit, F_N, as defined by Smith and Snyder [1979], and $\overline{|\Delta 2\theta|}$ was the average absolute magnitude of discrepancy between observed and calculated 2θ values for each reported hkℓ. N_{poss} was the number of diffraction lines allowed in the space group, up to the N^{th} observed and indexed line. Co-positional lines such as the cubic 221 and 300 are counted as one possible line.

Intensity measurements. It was found that samples which gave satisfactory intensity patterns usually had an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see Figure 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position. With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (see Figure 2). If the sample powder did not flow readily, or was prone to orient excessively, approximately 50 volume percent of finely ground silica-gel was added as a diluent. Occasionally, a rotating sample holder was used instead. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the strongest line.

As a check on reproducibility, each sample was mounted at least 3 times. The intensity values were determined for each of the mountings. Theta-compensating (variable divergence) slits were sometimes used to gather the intensity data. In that case, the average I(comp) for each spacing was converted to an equivalent fixed slit value, using the approximate equation:

$$I(\text{fixed}) = \frac{I(\text{comp})}{\sin\Theta}$$

The reported I^{rel} value for each observed spacing was the scaled average of the separate measurements, rounded to the nearest integer. The estimated standard deviation, σ, in the relative intensity values was calculated from the values of the five strongest lines, excluding the line with I =100.

$$\sigma_i^2 = \frac{1}{n-1} \sum_{j=1}^{n} (I_j^{rel}(k) - \langle I\rangle_j)^2$$

and

$$\sigma = \{\frac{1}{m} \sum_{i=1}^{m} \sigma_i^2\}^{\frac{1}{2}}$$

where

m is the number of strong lines (usually 5), and
n is the number of independent observations i, per line.

Where conversion of intensities for effects of theta-compensating slits was required, each σ_i was multiplied by the conversion factor

$$f = \frac{I(\text{comp})}{I(\text{fixed})}$$

Reference Intensity Ratio, $I/I_{corundum}$.

The reference intensity ratio, I/I_c, has been defined as the direct ratio of the intensity of the strongest reflection of a sample, to the intensity of the reflection 113 (hexagonal) of corundum (α-Al_2O_3) [Visser and de Wolff, 1964]. In this publication the ratios I/I_c were tabulated for copper Kα radiation, for a 1:1 mixture

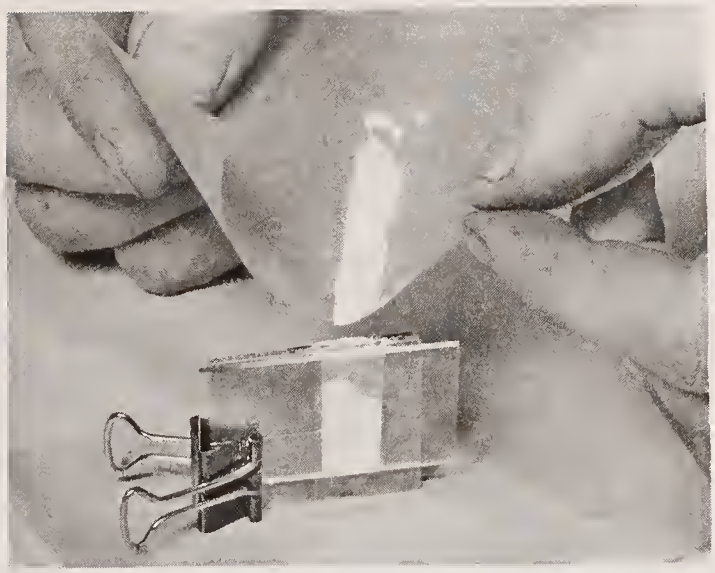

Figure 1.

Figure 2.

by weight of the sample and corundum. Occasionally I/I_c was not determined because it was not feasible.

A procedure has been adopted, to achieve greater statistical accuracy [Hubbard and Smith, 1977]. For any weight fractions of sample and corundum, x_s and x_c ($x_s = 1-x_c$), the intensities for reflection $\underline{h}$ of the sample and $\underline{k}$ of corundum were measured for several combinations of $\underline{h}$ and $\underline{k}$ usually within the same region of 2Θ, to provide indications of possible preferred orientation, extinction, or other systematic errors. The reference intensity ratio is then given by

$$\frac{I(h_o)}{I_c(113)} = \frac{x_c}{x_s} \cdot \frac{I_c^{rel}(\underline{k})}{I^{rel}(\underline{h})} \cdot \frac{I(\underline{h})}{I(\underline{k})}$$

and (h_o) indicates specifically which reflection was chosen for tabulation purposes. For each of our patterns, the reflection (h_o) will be the one with I = 100 since only copper radiation was used. Typically, at least 3 sets of reflections and 2 mountings of the mixture were used to obtain 6 or more values for the reference intensity ratio, I/I_c. These values yield the tabulated average $\langle I/I_c \rangle$. From these data, the estimated deviation, Δ, was obtained from

$$\Delta = \frac{\sum_{i=1}^{n} \left| (I/I_c)_i - \langle I/I_c \rangle \right|}{n}$$

where n is the number of measurements of the reference intensity ratio. The estimated deviation in the least significant figures is given in parentheses.

Format of tables. The printing of the data has been computerized. Superimposed reflections were treated in one of two ways. If a d-spacing had only two possible indices, an M was added to the d-spacing which was repeated on the next line, but with the second index. However, if there were more than two possible indices, a plus sign was used in like manner. In both cases, the composite intensity was printed only once and aligned with the first reflection. The symbol "1L" in the intensity column was used to indicate "less than 1".

UNITS

In this publication the Ångström unit (1Å = 100 pm) was selected for presentation of the d-spacings and lattice parameters to maintain consistency with (a) the earlier publications of Standard X-ray Diffraction Powder Patterns (Circular 539 volumes 1-10 and Monograph 25 sections 1-16), (b) the publications of the International Union of Crystallography: Acta Crystallographica and the Journal of Applied Crystallography, and (c) the continuing publication of cards and search manuals of the Powder Diffraction File (now consisting of over 33,000 entries). The PDF search manuals are based on the d-spacings in Å of the three strongest lines. Consistent with the choice of the Å unit for length, the volume of the unit cell is expressed in $Å^3$ ($1Å^3 = 1 \times 10^{-30}\ m^3$). Densities are reported in g/cm^3 ($1\ gm/cm^3 = 10^3\ kg/m^3$).

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Aluminum Borate, $Al_{18}B_4O_{33}$

CAS registry no.
12005-61-7

Sample
The sample was prepared by heating a 1:1 mixture of Al_2O_3 and H_3BO_3 together at 1250 °C. The compound was later annealed at 1500 °C.

Color
Colorless

Structure
Orthorhombic, Amam (63), $A2_1am$ (36), or Ama2 (40), Z = 1 [Scholze, 1956]. Baumann and Moore [1942] reported data for this phase. Although the lattice constants were in good agreement with NBS constants, their pattern does not index on the given cell.

Lattice constants of this sample

a = 7.6874(8) Å
b = 15.0127(15)
c = 5.6643(6)

a/b = 0.5121
c/b = 0.3773

Volume
653.70 $Å^3$

Density
(calculated) 2.685 g/cm^3

Figure of merit
F_{30} = 65.2(0.010,45)

Reference intensity
$I/I_{corundum}$ = 1.27(5)

Additional pattern
1. PDF card 9-248 [Scholze, 1956]

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CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
7.52	1	0 2 0	11.76
5.375	100	1 2 0	16.48
5.301	18	0 1 1	16.71
4.365	52	1 1 1	20.33
3.846	8	2 0 0	23.11
3.750M	16	0 4 0	23.71
3.750M		0 3 1	23.71
3.419	14	2 2 0	26.04
3.373M	42	1 4 0	26.40
3.373M		1 3 1	26.40
3.111	2	2 1 1	28.67
2.831	7	0 0 2	31.58
2.685M	41	2 4 0	33.35
2.685M		2 3 1	33.35
2.649	4	0 2 2	33.81
2.505	25	1 2 2	35.82
2.424	4	3 2 0	37.05
2.307	5	3 1 1	39.01
2.281	3	2 0 2	39.48
2.260	14	0 4 2	39.85
2.181	27	2 2 2	41.36
2.169	10	1 4 2	41.61
2.116M	21	3 4 0	42.69
2.116M		3 3 1	42.69
2.097	3	2 6 0	43.11
2.005	1L	0 7 1	45.18
1.9474	4	2 4 2	46.60
1.9415	2	1 7 1	46.75
1.9218	2	4 0 0	47.26
1.8733	5	0 1 3	48.56
1.8618	4	4 2 0	48.88
1.8424M	13	3 5 1	49.43
1.8424M		3 2 2	49.43
1.8196	12	1 1 3	50.09
1.7896	3	3 6 0	50.99
1.7776	5	2 7 1	51.36
1.7215	2	1 3 3	53.16
1.7105M	6	4 4 0	53.53
1.7105M		4 3 1	53.53
1.6852	14	2 6 2	54.40
1.5904	7	4 0 2	57.94
1.5650M	6	1 5 3	58.97
1.5650M		0 8 2	58.97
1.5564M	3	4 5 1	59.33
1.5564M		4 2 2	59.33

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
1.5330	2	1 8 2	60.33
1.5130M	19	3 6 2	61.21
1.5130M		3 1 3	61.21
1.4764+	3	5 1 1	62.90
1.4764+		2 5 3	62.90
1.4643	2	4 4 2	63.48
1.4496	7	2 8 2	64.20
1.4159	9	0 0 4	65.92
1.3982	2	2 10 0	66.86
1.3876	1	4 7 1	67.44
1.3694	2	1 2 4	68.46
1.3560	3	3 5 3	69.23
1.3425M	3	4 8 0	70.03
1.3425M		4 6 2	70.03
1.3299+	10	5 2 2	70.79
1.3299+		2 7 3	70.79
1.3067	6	1 10 2	72.24
1.2953	2	3 10 0	72.98
1.2810	1	6 0 0	73.93
1.2716	1	5 4 2	74.57
1.2631	1	6 2 0	75.16
1.2533M	7	2 10 2	75.85
1.2533M		2 4 4	75.85
1.2513	6	0 12 0	75.99
1.2339	2	1 9 3	77.26
1.2296	1	4 9 1	77.58
1.2231	1	3 2 4	78.07
1.2129+	1	4 8 2	78.85
1.2129+		6 4 0	78.85
1.1890+	1	5 6 2	80.76
1.1890+		2 9 3	80.76
1.1770	2	3 4 4	81.76

Ammonium Borate Hydrate, $NH_4B_5O_8 \cdot 4H_2O$

Synonyms
1. Ammonium pentaborate tetrahydrate
2. APT

CAS registry no.
12229-12-8

Sample
The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from an aqueous solution at room temperature.

Color
Colorless

Structure
Orthorhombic, Bba2 (41), Z = 4 [Cook and Jaffe, 1957; Clark and Christ, 1959].

Lattice constants of this sample

a = 11.033(3) Å
b = 11.332(3)
c = 9.238(3)

a/b = 0.9736
c/b = 0.8152

Volume
1155.0 $Å^3$

Density
(calculated) 1.565 g/cm^3

Figure of merit
F_{30} = 57.2 (0.014,38)

Reference intensity
$I/I_{corundum}$ = 1.08(6)

Additional pattern
1. PDF card 12-638 [Clark and Christ, 1959]

References
Clark, J. R. and Christ, C. L. (1959). Amer. Mineral. 44, 1150.
Cook, W. R., Jr. and Jaffe, H. (1957). Acta Crystallogr. 10, 705.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.00	63	1 1 1	14.74
5.67	12	0 2 0	15.63
5.52	46	2 0 0	16.04
4.951	2	2 1 0	17.90
4.617	7	0 0 2	19.21
4.427	1	1 2 1	20.04
3.544	80	2 0 2	25.11
3.383	100	2 1 2	26.32
3.334	11	1 3 1	26.72
3.271	9	3 1 1	27.24
3.003	4	2 2 2	29.73
2.926	7	3 2 1	30.53
2.868	4	1 1 3	31.16
2.834	31	0 4 0	31.54
2.760	2	4 0 0	32.41
2.680	2	4 1 0	33.41
2.627	5	1 2 3	34.10
2.586	1	2 3 2	34.66
2.533	8	3 3 1	35.41
2.479	1L	4 2 0	36.20
2.414	1	0 4 2	37.21
2.367	4	4 0 2	37.98
2.332	4	1 3 3	38.58
2.317	9	4 1 2	38.83
2.312M	9	3 1 3	38.93
2.312M		0 0 4	38.93
2.212	8	2 4 2	40.75
2.182	16	3 4 1	41.35
2.178	16	3 2 3	41.43
2.158	4	1 5 1	41.83
2.138	3	0 2 4	42.24
2.107	7	5 1 1	42.88
2.095M	2	2 5 0	43.14
2.095M		2 1 4	43.14
2.048	2	1 4 3	44.18
2.007M	7	5 2 1	45.15
2.007M		4 3 2	45.15
1.909	6	2 5 2	47.59
1.888M	2	3 5 1	48.16
1.888M		0 6 0	48.16
1.856	4	2 3 4	49.03
1.817	4	4 4 2	50.16
1.7998M	2	1 5 3	50.68
1.7998M		1 1 5	50.68
1.7715M	3	5 1 3	51.55

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
1.7715M		4 0 4	51.55
1.7506M	3	4 5 0	52.21
1.7506M		4 1 4	52.21
1.7102M	2	5 4 1	53.54
1.7102M		5 2 3	53.54
1.7029	2	2 4 4	53.79
1.6533M	1	6 3 0	55.54
1.6533M		3 6 1	55.54
1.6206	1L	5 3 3	56.76
1.5780	1	1 7 1	58.44
1.5427	1	6 4 0	59.91

Ammonium Nickel Sulfate Hydrate, $(NH_4)_2Ni(SO_4)_2 \cdot 6H_2O$

CAS registry no.
51287-85-5

Sample
The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color
Strong bluish green

Structure
Monoclinic, $P2_1/a$ (14), Z = 2. The structure was determined by Grimes et al. [1963] and by Montgomery and Lingafelter [1964]. It is isostructural with other "Tutton" salts [Tutton, 1916].

Lattice constants of this sample

a = 9.1862(15) Å
b = 12.468(2)
c = 6.2423(10)
β = 106.93(2)°

a/b = 0.7368
c/b = 0.5007

Volume
684.0 $Å^3$

Density
(calculated) 1.918 g/cm^3

Figure of merit
F_{30} = 63.7(0.012,38)

Reference intensity
$I/I_{corundum}$ = 0.92(5)

Additional pattern
1. PDF card 12-454 [Institute of Physics, Cardiff, Wales]

References

Grimes, N. W., Kay, H. F., and Webb, M. W. (1963). Acta Crystallogr. 16, 823.
Montgomery, H. and Lingafelter, E. C. (1964). Acta Crystallogr. 17, 1478.
Tutton, A. E. (1916). Trans. Roy. Soc. London Ser. A 216, 1.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±5	hkℓ	2θ(°)
7.19	4	1 1 0	12.30
6.24	30	0 2 0	14.19
5.98	14	0 0 1	14.80
5.388	36	0 1 1	16.44
5.248	7	-1 1 1	16.88
5.090	20	1 2 0	17.41
4.397	19	2 0 0	20.18
4.316	21	0 2 1	20.56
4.243	36	-1 2 1	20.92
4.166	100	-2 0 1	21.31
4.147	66	2 1 0	21.41
3.952	6	-2 1 1	22.48
3.757	88	1 3 0	23.66
3.586	16	1 2 1	24.81
3.466	4	-2 2 1	25.68
3.410	14	0 3 1	26.11
3.376	18	-1 3 1	26.38
3.119	20	0 4 0	28.60
3.037	32	2 1 1	29.39
3.027	44	-1 1 2	29.49
2.943	4	-2 3 1	30.35
2.913	4	-3 1 1	30.67
2.903	5	0 1 2	30.77
2.892	6	-2 0 2	30.89
2.853	6	3 1 0	31.33
2.816	6	-2 1 2	31.75
2.796	28	2 2 1	31.98
2.790	26	-1 2 2	32.05
2.742	3	-1 4 1	32.63
2.703	8	-3 2 1	33.12
2.651	1	3 2 0	33.79
2.623	2	-2 2 2	34.16
2.550	6	1 1 2	35.17
2.541M	11	2 4 0	35.29
2.541M		1 4 1	35.29
2.501	7	2 3 1	35.88
2.430	25	-3 3 1	36.96
2.395	3	3 3 0	37.52
2.374	2	-2 3 2	37.86
2.302	2	0 5 1	39.10
2.208M	16	1 3 2	40.84
2.208M		2 4 1	40.84
2.166+	7	1 5 1	41.67
2.166+		4 1 0	41.67
2.156M	9	0 4 2	41.86
2.156M		2 1 2	41.86
2.134	9	3 4 0	42.31
2.120	6	-2 4 2	42.62
2.072	10	4 2 0	43.64
2.052	2	-2 0 3	44.09
2.049	2	-1 1 3	44.17
2.024	3	-2 1 3	44.74
2.005	1	-4 3 1	45.19
1.990	4	0 0 3	45.54
1.975	2	-4 2 2	45.92
1.963	4	0 6 1	46.22
1.956	3	-1 6 1	46.39
1.950M	2	2 5 1	46.53
1.950M		-2 2 3	46.53
1.942M	2	4 3 0	46.73

d(Å)	I^{rel} $\sigma = \pm 5$	hkℓ	2θ(°)
1.942M		-3 4 2	46.73
1.915	7	0 5 2	47.43
1.905	10	-3 1 3	47.71
1.899	10	3 5 0	47.87
1.878M	3	1 6 1	48.44
1.878M		2 6 0	48.44
1.8575	7	-1 3 3	49.00
1.8389	6	-2 3 3	49.53
1.8179	3	-5 1 1	50.14
1.8095M	5	4 2 1	50.39
1.8095M		1 1 3	50.39
1.7949M	10	0 3 3	50.83
1.7949M		4 4 0	50.83
1.7919	8	2 4 2	50.92
1.7632	2	-5 2 1	51.81
1.7588	4	-3 5 2	51.95
1.7401	4	5 1 0	52.55
1.7288M	2	-1 6 2	52.92
1.7288M		-1 4 3	52.92
1.7176	5	3 5 1	53.29
1.7132	6	-2 4 3	53.44
1.7052	2	0 6 2	53.71
1.6855M	5	-4 2 3	54.39
1.6855M		-4 5 1	54.39
1.6826	4	3 3 2	54.49
1.6750	3	1 3 3	54.76

Ammonium Sulfate, $(NH_4)_2S_2O_3$

Synonym
1. Ammonium thiosulfate

CAS registry no.
7783-18-8

Sample
The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color
Colorless

Structure
Monoclinic, C2/m (12), Z = 4. The structure was determined by Brunt [1946]. A line at $2\theta = 23.06$ with I = 4, could not be indexed.

Lattice constants of this sample

a = 10.2233(15) Å
b = 6.4956(9)
c = 8.8074(10)
β = 94.66(1)°

a/b = 1.5739
c/b = 1.3559

Volume
582.93 $Å^3$

Density
(calculated) 1.689 g/cm^3

Figure of merit
F_{30} = 91.0(0.010,34)

Reference intensity
$I/I_{corundum}$ = 0.94(3)

Additional pattern
1. PDF card 1-844 [Hanawalt et al., 1938]

References
Brunt, N. A. (1946). Diss. Leiden pp. 64.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±8	hkℓ	2θ(°)
5.480	16	1 1 0	16.16
5.093	44	2 0 0	17.40
4.741	93	-1 1 1	18.70
4.553	100	1 1 1	19.48
4.386	76	0 0 2	20.23
4.257	18	2 0 1	20.85
3.501	16	-1 1 2	25.42
3.469	14	-2 0 2	25.66
3.353	32	1 1 2	26.56
3.248	18	0 2 0	27.44
3.199	28	2 0 2	27.87
3.046	22	0 2 1	29.30
3.010	74	3 1 0	29.66
2.925	8	0 0 3	30.54
2.915	9	-3 1 1	30.65
2.785	9	3 1 1	32.11
2.739	6	2 2 0	32.67
2.629M	62	-2 0 3	34.07
2.629M		-1 1 3	34.07
2.612	32	0 2 2	34.31
2.582	14	2 2 1	34.71
2.569	13	-3 1 2	34.90
2.547	8	4 0 0	35.21
2.536	8	1 1 3	35.36
2.500	2	-4 0 1	35.89
2.453	5	2 0 3	36.61
2.402	6	3 1 2	37.41
2.395	6	4 0 1	37.52
2.371	20	-2 2 2	37.92
2.286	6	-4 0 2	39.39
2.280	6	2 2 2	39.50
2.195	6	0 0 4	41.09
2.178	6	-3 1 3	41.42
2.129	3	4 0 2	42.42
2.118	2	1 3 0	42.65
2.078	4	-2 0 4	43.51
2.0688M	5	-1 1 4	43.72
2.0688M		-1 3 1	43.72
2.0510	4	1 3 1	44.12
2.0444	4	-2 2 3	44.27
2.0270	2	3 1 3	44.67
2.0065	6	1 1 4	45.15
1.9824	2	-4 2 1	45.73
1.9582M	7	2 0 4	46.33
1.9582M		2 2 3	46.33
1.9451	3	5 1 0	46.66
1.9271	3	4 2 1	47.12
1.8946	3	1 3 2	47.98
1.8686M	3	-4 2 2	48.69
1.8686M		5 1 1	48.69
1.8368	2	-3 1 4	49.59
1.8319	2	-5 1 2	49.73
1.8261	4	3 3 0	49.90
1.8186	12	0 2 4	50.12
1.8031	7	-3 3 1	50.58

d(Å)	I^{rel} $\sigma = \pm 8$	hkℓ	2θ(°)
1.7814	2	4 2 2	51.24
1.7559	5	0 0 5	52.04
1.7294M	10	-1 3 3	52.90
1.7294M		5 1 2	52.90
1.7159	3	3 1 4	53.35
1.7117	4	-3 3 2	53.49
1.7052	6	-4 2 3	53.71
1.7023M	6	-2 0 5	53.81
1.7023M		1 3 3	53.81
1.6933M	6	-1 1 5	54.12
1.6933M		-6 0 1	54.12
1.6801	4	-5 1 3	54.58
1.6775	4	2 2 4	54.67
1.6599	2	3 3 2	55.30
1.6508	2	1 1 5	55.63
1.6196	1	2 0 5	56.80
1.6066	1	4 2 3	57.30
1.5967	1	0 4 1	57.69
1.5809	2	-3 3 3	58.32
1.5665	4	-3 1 5	58.91

Synonym
Ammonium persulfate

Sample
The sample was from Fisher Scientific Co. Fair Lawn, NJ. The sample was hygroscopic.

Color
Colorless

Structure
Monoclinic, $P2_1/n(14)$, Z = 2. The structure of $(NH_4)_2S_2O_8$ has been determined by Zachariasen and Mooney [1934] and refined by Sivertsen and Sorum [1969].

Lattice constants of this sample
a = 7.829(2)
b = 8.0075(14)
c = 6.1483(12)
β = 95.12(2)°

a/b = 0.9777
c/b = 0.7678

Volume
383.90 $Å^3$

Density
(calculated) 1.974 g/cm^3

Figure of merit
F_{30} = 41.9(0.015,48)

Additional pattern
1. PDF card 11-551 [University College, Cardiff, Wales]

References

Sivertsen, B. K. and Sorum, H. (1969) Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 130, 449.
Zachariasen, W. H. and Mooney, R. C. L. (1934) Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 88, 63.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±6	hkℓ	2θ(°)
5.583	42	1 1 0	15.86
5.038	62	-1 0 1	17.59
4.862	14	0 1 1	18.23
4.621	10	1 0 1	19.19
4.261	12	-1 1 1	20.83
3.996M	50	0 2 0	22.23
3.996M		1 1 1	22.23
3.560	62	1 2 0	24.99
3.501	69	2 1 0	25.42
3.347	100	0 2 1	26.61
3.154	50	-2 1 1	28.27
3.063	16	0 0 2	29.13
3.027	2	1 2 1	29.49
2.945	19	2 1 1	30.33
2.860	18	0 1 2	31.25
2.761	2	-1 1 2	32.40
2.606	6	-2 2 1	34.39
2.526	3	1 3 0	35.51
2.483	28	2 2 1	36.15
2.475M	25	-3 0 1	36.27
2.475M		3 1 0	36.27
2.433	6	0 2 2	36.92
2.403	13	-2 1 2	37.39
2.370	4	-1 2 2	37.93
2.309M	8	1 3 1	38.97
2.309M		2 0 2	38.97
2.220	10	2 1 2	40.61
2.204	8	2 3 0	40.92
2.181	2	3 2 0	41.36
2.041	16	2 3 1	44.35
2.019	2	-1 0 3	44.85
2.012	4	0 3 2	45.01
2.007	6	3 2 1	45.14
1.978M	5	0 1 3	45.84
1.978M		-1 3 2	45.84
1.940	3	1 4 0	46.80
1.933	8	1 0 3	46.97
1.921	4	1 3 2	47.27
1.8791	4	1 1 3	48.40
1.8625	6	3 3 0	48.86
1.8424	2	-3 2 2	49.43
1.8368	6	1 4 1	49.59
1.8145	2	-3 3 1	50.24
1.7805	8	2 4 0	51.27
1.7660	2	4 1 1	51.72
1.7509	3	3 3 1	52.20
1.7459	3	2 3 2	52.36
1.7285	2	-2 4 1	52.93
1.7221	11	-4 2 1	53.14
1.6750	2	0 4 2	54.76
1.6549	2	-1 4 2	55.48
1.6505	4	4 2 1	55.64
1.6000	3	2 2 3	57.56

Cadmium Bromate Hydrate, $Cd(BrO_3)_2 \cdot 2H_2O$

Synonym
1. Cadmium bromate dihydrate

CAS registry no.
19320-65-1

Sample
The sample was prepared by dissolving anhydrous $Cd(BrO_3)_2$ in water and letting it dry. The sample was then washed.

Color
Light orange yellow.

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was studied by Garcia-Blanco and Perales [1963].

Lattice constants of this sample

a = 9.2417(10) Å
b = 12.5015(13)
c = 6.1762(6)

a/b = 0.7392
c/b = 0.4940

Volume
713.57 $Å^3$

Density
(calculated) 3.763 g/cm^3

Figure of merit
F_{30} = 62.5(0.012,39)

Reference intensity
$I/I_{corundum}$ = 2.9(2)

Additional pattern
1. PDF card 1-0353 (labelled monohydrate) [Hanawalt et al. 1938]

References
Garcia-Blanco, S. and Perales, A. (1963). Acta Crystallogr. 16, A34.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
6.24	22	0 2 0	14.18
5.538	28	0 1 1	15.99
5.172	1	1 2 0	17.13
5.131	1	1 0 1	17.27
4.746	4	1 1 1	18.68
4.621	1	2 0 0	19.19
4.397	100	0 2 1	20.18
3.969	4	1 2 1	22.38
3.799	2	1 3 0	23.40
3.714	15	2 2 0	23.94
3.700	15	2 0 1	24.03
3.546	21	2 1 1	25.09
3.453	22	0 3 1	25.78
3.236	11	1 3 1	27.54
3.184	26	2 2 1	28.00
3.123	12	0 4 0	28.56
3.091M	24	2 3 0	28.86
3.091M		0 0 2	28.86
2.996	5	0 1 2	29.80
2.990	5	3 1 0	29.86
2.959	3	1 4 0	30.18
2.929	1L	1 0 2	30.50
2.851	14	1 1 2	31.35
2.769M	16	0 2 2	32.31
2.769M		2 3 1	32.31
2.692	5	3 1 1	33.25
2.669	3	1 4 1	33.55
2.651	3	1 2 2	33.79
2.590	3	2 4 0	34.61
2.568	2	2 0 2	34.91
2.514	10	2 1 2	35.68
2.480	4	0 3 2	36.19
2.477	3	3 3 0	36.24
2.396	5	1 3 2	37.51
2.389	6	2 4 1	37.62
2.375	7	2 2 2	37.85
2.318	5	0 5 1	38.81
2.273	8	4 1 0	39.62
2.248	5	1 5 1	40.07
2.196M	22	0 4 2	41.07
2.196M		3 4 0	41.07
2.181	5	3 0 2	41.36
2.164	2	4 0 1	41.70
2.148	3	3 1 2	42.02
2.137	6	1 4 2	42.25

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
2.133	5	4 1 1	42.35
2.083	4	0 6 0	43.41
2.071	11	2 5 1	43.68
2.067	10	3 4 1	43.77
2.044	5	4 2 1	44.27
2.033M	9	1 6 0	44.54
2.033M		0 1 3	44.54
2.011	3	1 0 3	45.05
1.9845M	4	1 1 3	45.68
1.9845M		2 4 2	45.68
1.9747	2	0 6 1	45.92
1.9443	10	0 5 2	46.68
1.9322M	3	3 3 2	46.99
1.9322M		1 6 1	46.99
1.9195	4	4 3 1	47.32
1.9122	5	1 2 3	47.51
1.9013	1	1 5 2	47.80
1.8810	1	2 0 3	48.35
1.8597	1	2 1 3	48.94
1.8501	2	4 0 2	49.21
1.8462	1	0 3 3	49.32
1.8285	1	5 1 0	49.83
1.8159	5	2 6 1	50.20
1.8008	3	2 2 3	50.65
1.7886	4	3 4 2	51.02
1.7789	3	4 4 1	51.32
1.7547M	1	1 7 0	52.08
1.7547M		5 1 1	52.08
1.7194	2	0 4 3	53.23
1.7147M	4	0 7 1	53.39
1.7147M		2 3 3	53.39
1.7040	2	5 2 1	53.75
1.6967+	3	4 5 0	54.00
1.6967+		3 1 3	54.00
1.6904+	6	1 4 3	54.22
1.6904+		5 3 0	54.22
1.6872	5	1 7 1	54.33
1.6665	2	2 7 0	55.06
1.6621	3	3 6 1	55.22
1.6511	1	3 2 3	55.62
1.6432	3	3 5 2	55.91
1.6362	2	4 5 1	56.17
1.6298	3	5 3 1	56.41
1.6177	1	2 6 2	56.87
1.6110	3	2 4 3	57.13
1.6084	3	2 7 1	57.23
1.5921	2	4 4 2	57.87
1.5901M	2	5 4 0	57.95
1.5901M		0 5 3	57.95
1.5831	4	3 3 3	58.23
1.5735	1	5 1 2	58.62
1.5633	2	0 8 0	59.04
1.5457M	2	0 7 2	59.78
1.5457M		3 7 0	59.78
1.5413M	3	1 8 0	59.97
1.5413M		5 4 1	59.97
1.5373M	2	5 2 2	60.14
1.5373M		4 0 3	60.14
1.5327	3	0 1 4	60.34
1.5243	1	1 7 2	60.71
1.5146	2	0 8 1	61.14
1.5117	3	1 1 4	61.27
1.5030	1	2 5 3	61.66
1.5006M	1	3 4 3	61.77
1.5006M		4 6 1	61.77
1.4989M	1	0 2 4	61.85
1.4989M		3 7 1	61.85
1.4945M	1	1 8 1	62.05
1.4945M		6 0 1	62.05
1.4866M	2	4 5 2	62.42
1.4866M		5 5 0	62.42
1.4838	3	6 1 1	62.55
1.4657	3	2 7 2	63.41
1.4641M	3	2 0 4	63.49
1.4641M		0 6 3	63.49
1.4482	3	0 3 4	64.27
1.4445M	2	5 5 1	64.45
1.4445M		6 3 0	64.45
1.4303	2	1 3 4	65.17
1.4255	1	2 2 4	65.42
1.4130M	1	4 7 0	66.07
1.4130M		3 5 3	66.07
1.4070	1	6 3 1	66.39
1.3942M	2	0 8 2	67.08
1.3942M		3 8 0	67.08

Calcium Sulfate Hydrate (Gypsum), $CaSO_4 \cdot 2H_2O$

Synonym
1. Calcium sulfate dihydrate

CAS registry no.
10101-41-4

Sample
The sample was prepared by adding H_2SO_4 to a water solution of $Ca(NO_3)_2$. The precipitate was filtered out, washed in water, and bottled while moist. The crystals were dried immediately before use, and care was taken to prevent dehydration.

Color
Colorless

Structure
Monoclinic, C2/c (15), Z = 4. The structure was determined by Wooster [1936] and refined by Atoji and Rundle [1958].

Lattice constants of this sample

a = 6.2845(11) Å
b = 15.2079(15)
c = 5.6776(7)
β = 114.09(1)°

a/b = 0.4132
c/b = 0.3733

Volume
495.37 $Å^3$

Density
(calculated) 2.308 g/cm^3

Figure of merit
F_{30} = 47.4(0.013,49)

Reference intensity
$I/I_{corundum}$ = 1.83(4)

Additional patterns
1. PDF card 6-0046 [F. H. Gillery, Pennsylvania State University, University Park, PA]
2. PDF card 21-816 [Technisch Physische Dienst, Delft, Holland]

References
Atoji, M. and Rundle, R. E. (1958). J. Chem. Phys. 29, 1306.
Wooster, W. A. (1936). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 94, 375.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
7.63	100	0 2 0	11.59
4.283	98	0 2 1	20.72
3.799M	17	0 4 0	23.40
3.799M		1 3 0	23.40
3.172	4	1 1 1	28.11
3.065	74	0 4 1	29.11
2.873	47	-2 2 1	31.10
2.789	10	-1 1 2	32.07
2.732	2	1 3 1	32.75
2.685M	34	1 5 0	33.35
2.685M		2 2 0	33.35
2.597	6	-1 5 1	34.51
2.534	2	0 6 0	35.39
2.495	11	-2 0 2	35.97
2.476	1	-1 3 2	36.25
2.452	6	0 2 2	36.62
2.406	4	-2 4 1	37.35
2.291	1L	2 4 0	39.29
2.219	15	1 5 1	40.63
2.142	2	0 4 2	42.15
2.086	24	-2 4 2	43.34
2.074M	15	-1 5 2	43.60
2.074M		-3 1 1	43.60
2.048	6	1 1 2	44.18
2.032	1L	1 7 0	44.56
1.992	4	-1 7 1	45.51
1.963	3	-2 6 1	46.22
1.8998M	16	0 8 0	47.84
1.8998M		2 6 0	47.84
1.8795	12	2 4 1	48.39
1.8650	3	-1 1 3	48.79
1.8118	13	0 6 2	50.32
1.7995	6	-2 2 3	50.69
1.7844	9	0 8 1	51.15
1.7785	12	-2 6 2	51.33
1.7093	1	1 5 2	53.57
1.6846	3	0 2 3	54.42
1.6640	6	-2 4 3	55.15
1.6456	4	2 6 1	55.82
1.6209+	9	-2 8 1	56.75
1.6209+		1 9 0	56.75
1.6005	1	-1 9 1	57.54
1.5846	4	2 8 0	58.17
1.5327	2	0 8 2	60.34
1.5209+	1	0 10 0	60.86

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ	2θ(°)
1.5209+		-4 2 2	60.86
1.5119	1	-2 8 2	61.26
1.4982	1L	1 9 1	61.88
1.4947	1L	-2 6 3	62.04
1.4591+	3	-3 7 2	63.73
1.4591+		0 10 1	63.73
1.4392	5	-4 4 1	64.72
1.4354	3	3 7 0	64.91
1.4278M	2	2 8 1	65.30
1.4278M		0 6 3	65.30
1.4178	3	-2 0 4	65.82
1.4015	2	-4 2 3	66.68
1.3657M	5	2 6 2	68.67
1.3657M		-2 10 1	68.67
1.3440M	1	1 11 0	69.94
1.3440M		2 10 0	69.94
1.3324	2	-1 11 1	70.64
1.3262	4	-2 8 3	71.02
1.3234	4	-4 6 2	71.19
1.2785	1	0 8 3	74.10
1.2722	1L	1 11 1	74.53
1.2674	1L	0 12 0	74.86
1.2481M	3	4 6 0	76.22
1.2481M		-4 0 4	76.22
1.2441	2	2 10 1	76.51
1.2336	3	2 8 2	77.28
1.2309+	2	-4 2 4	77.48
1.2309+		0 12 1	77.48

Calcium Tin Oxide, $CaSnO_3$

Synonym
1. Calcium stannate

CAS registry no.
12013-46-6

Sample
The sample was obtained from CERAC, Inc. Milwaukee, WI. The material was heated to 800 °C for one hour. A small amount of SnO_2 was present in the sample.

Color
White

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure of $CaSnO_3$ was studied by Smith and Welch [1960].

Lattice constants of this sample

a = 5.6615(5) Å
b = 7.8825(7)
c = 5.5162(5)

a/b = 0.7182
c/b = 0.6998

Volume
246.17 $Å^3$

Density
(calculated) 5.579 g/cm^3

Figure of merit
F_{30} = 55.5(0.011,51)

Reference intensity
$I/I_{corundum}$ = 6.5(4)

Additional patterns
1. PDF card 3-755 [H. D. Megaw, Philips Lamps Ltd.]
2. Coughanour et al. [1955]

References

Coughanour, L. W., Roth, R. S., Marzullo, S., and Sennett, F. E. (1955). J. Res. Nat. Bur. Stand. 54, No. 3, 149.
Smith, A. J. and Welch, A. J. E. (1960). Acta. Crystallogr. 13, 653.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
3.943	60	0 2 0	22.53
3.531	2	1 1 1	25.20
2.830	26	2 0 0	31.59
2.789	100	1 2 1	32.07
2.758	23	0 0 2	32.44
2.518	1L	2 0 1	35.62
2.480	1	1 0 2	36.19
2.398	1	2 1 1	37.47
2.371	3	0 3 1	37.91
2.366	3	1 1 2	38.00
2.298	3	2 2 0	39.17
2.259	3	0 2 2	39.87
2.188	2	1 3 1	41.22
2.122	1	2 2 1	42.56
2.099	1L	1 2 2	43.06
1.9751	32	2 0 2	45.91
1.9714	29	0 4 0	46.00
1.9256	1	2 3 0	47.16
1.9168	1	2 1 2	47.39
1.8183	1L	2 3 1	50.13
1.8038	1L	1 3 2	50.56
1.7853	7	3 0 1	51.12
1.7638	19	1 4 1	51.79
1.7484	4	1 0 3	52.28
1.7076	1	1 1 3	53.63
1.6266	15	3 2 1	56.53
1.6177	12	2 4 0	56.87
1.6030	15	0 4 2	57.44
1.5984	23	1 2 3	57.62
1.5420M	1L	1 4 2	59.94
1.5420M		2 0 3	59.94
1.4766	1	3 3 1	62.89
1.4155	2	4 0 0	65.94
1.3951	2	2 4 2	67.03
1.3788	10	0 0 4	67.93
1.3393M	1L	1 0 4	70.22
1.3393M		3 3 2	70.22
1.3362	1	2 5 1	70.41
1.3320	2	4 2 0	70.66
1.3301M	2	1 5 2	70.78
1.3301M		2 3 3	70.78
1.3231	4	3 4 1	71.21
1.3173	2	3 0 3	71.57
1.3082	2	1 4 3	72.15
1.3021	1	0 2 4	72.54
1.2592	2	4 0 2	75.43
1.2489	7	3 2 3	76.16
1.2466M	9	1 6 1	76.33
1.2466M		4 3 0	76.33
1.2398	3	2 0 4	76.82
1.2324	1L	2 5 2	77.37
1.2247	1L	2 1 4	77.95
1.2144	1L	2 4 3	78.74
1.1994	2	4 2 2	79.92
1.1966	2	0 5 3	80.14

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
1.1916	1	2 6 0	80.55
1.1861	1	0 6 2	81.00
1.1825	3	2 2 4	81.30
1.1708	1L	1 5 3	82.28
1.1499	2	4 4 0	84.12
1.1358	1L	4 3 2	85.41
1.1300	2	0 4 4	85.95
1.1092	1	5 0 1	87.97
1.0948	2	3 4 3	89.43
1.0939	2	2 6 2	89.53

Cerium Nitrate Hydrate, $Ce(NO_3)_3 \cdot 6H_2O$

Synonym
1. Cerous nitrate hexahydrate

CAS registry no.
10294-41-4

Sample
The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color
Colorless

Structure
Triclinic, $P\bar{1}(2)$, Z = 2. The structure of $Ce(NO_3)_3 \cdot 6H_2O$ was studied by Iveronova et al. [1955].

Lattice constants of this sample

a = 8.905(2) Å
b = 10.683(3)
c = 6.6182(14)
α = 101.18(2)°
β = 102.19(2)
γ = 87.89(2)

a/b = 0.8336
c/b = 0.6195

Volume
603.7 $Å^3$

Density
(calculated 2.389 g/cm^3

Figure of merit
F_{30} = 45.8(0.013,51)

Reference intensity
$I/I_{corundum}$ = 0.44(3)

Additional pattern
1. PDF card 14-3 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Ivernova, V. I., Tarasova, V. P., Zolina, Z. K., Markhasin, G. V., and Sukhodereva, I. M. (1955). Zh. Fiz. Khim. 29, 314.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±5	hkℓ	2θ(°)
8.70	21	1 0 0	10.16
6.71	85	-1 1 0	13.19
6.37	60	0 0 1	13.90
5.96	76	0 -1 1	14.85
5.73	54	-1 0 1	15.44
5.437	42	-1 -1 1	16.29
5.245	42	0 2 0	16.89
5.024	44	0 1 1	17.64
4.701	100	-1 1 1	18.86
4.487M	39	0 -2 1	19.77
4.487M		1 2 0	19.77
4.358	46	2 0 0	20.36
4.017	22	2 1 0	22.11
4.001	27	-2 0 1	22.20
3.890	14	-2 -1 1	22.84
3.770	19	1 -2 1	23.58
3.711	6	0 2 1	23.96
3.576	4	-1 2 1	24.88
3.493	2	0 3 0	25.48
3.375	28	-2 -2 1	26.39
3.341M	21	0 -3 1	26.66
3.341M		2 2 0	26.66
3.247M	50	-1 3 0	27.45
3.247M		-1 -1 2	27.45
3.237M	33	1 3 0	27.53
3.237M		-1 -3 1	27.53
3.213	37	0 -1 2	27.74
3.175	15	0 0 2	28.08
3.048	14	2 1 1	29.28
3.013M	25	1 -3 1	29.63
3.013M		-2 2 1	29.63
3.002	28	-1 -2 2	29.74
2.979	29	0 -2 2	29.97
2.913	45	-1 1 2	30.67
2.892M	47	-2 -1 2	30.89
2.892M		0 1 2	30.89
2.875	11	-3 0 1	31.08
2.864	11	-2 0 2	31.20
2.839	31	0 3 1	31.49
2.832M	28	-3 -1 1	31.57
2.832M		1 -1 2	31.57
2.802M	11	1 0 2	31.91
2.802M		-3 1 0	31.91
2.794M	15	-2 -3 1	32.01
2.794M		3 1 0	32.01
2.715+	21	-3 1 1	32.96
2.715+		-2 -2 2	32.96
2.663M	19	1 -2 2	33.63
2.663M		2 2 1	33.63
2.651	35	-2 1 2	33.78
2.620	28	0 4 0	34.19
2.611M	30	-3 -2 1	34.32
2.611M		0 -3 2	34.32
2.550	19	-1 -4 1	35.16
2.542	14	-3 2 0	35.28

d(Å)	I^{rel} σ = ±5	hkℓ	2θ(°)
2.533	18	3 2 0	35.41
2.527M	24	-1 2 2	35.49
2.527M		2 -3 1	35.49
2.490	18	-2 3 1	36.04
2.452	20	3 0 1	36.62
2.440	15	1 -4 1	36.80
2.424	13	-2 -3 2	37.05
2.405	13	-3 0 2	37.36
2.393	5	1 -3 2	37.56
2.359	6	2 -1 2	38.12
2.352	12	-2 2 2	38.24
2.316M	23	-2 -4 1	38.85
2.316M		-3 -3 1	38.85
2.313M	26	-3 -2 2	38.91
2.313M		1 2 2	38.91
2.291	32	3 -2 1	39.30
2.280	31	2 3 1	39.49
2.265	14	2 -2 2	39.77
2.249M	28	-1 -4 2	40.06
2.249M		-2 4 0	40.06
2.243M	24	-1 4 1	40.17
2.243M		0 -4 2	40.17
2.227	5	3 3 0	40.47
2.204M	19	-1 -1 3	40.91
2.204M		-4 0 1	40.91
2.184	13	-4 -1 1	41.31
2.159+	27	1 4 1	41.80
2.159+		3 2 1	41.80
2.153M	27	0 3 2	41.92
2.153M		-1 -2 3	41.92
2.137	22	-3 3 1	42.26
2.129M	26	-4 1 1	42.43
2.129M		4 1 0	42.43
2.116M	35	0 0 3	42.70
2.116M		0 -5 1	42.70
2.107	28	0 -2 3	42.89
2.088	20	2 -3 2	43.29
2.081	20	-2 0 3	43.44
2.077M	21	-3 2 2	43.53
2.077M		-4 -2 1	43.53
2.053	11	-2 3 2	44.08
2.039	22	-1 5 0	44.39
2.035M	17	1 5 0	44.49
2.035M		2 2 2	44.49
2.024+	6	1 -5 1	44.74
2.024+		1 3 2	44.74
2.012	3	-4 2 0	45.01
1.999	19	-4 0 2	45.33
1.987M	8	-4 2 1	45.63
1.987M		0 -3 3	45.63
1.973	10	-2 1 3	45.97

CAS registry no.
12006-79-0

Sample
The sample was obtained from Cerac, Menomonee Falls, WI.

Color
Metallic gray

Structure
Orthorhombic, Cmcm (63), Z = 4. The structure was determined by Kiessling [1949].

Lattice constants of this sample

a = 2.9663(4) Å
b = 7.8666(10)
c = 2.9322(5)

a/b = 0.3771
c/b = 0.3727

Volume
68.422 $Å^3$

Density
(calculated) 6.097 g/cm^3

Figure of merit
F_{19} = 62.9(0.013,24)

Reference intensity
$I/I_{corundum}$ = 1.22(8)

Polymorphism
Papesch et al., [1973] also observed a tetragonal low temperature form of CrB with 52-56 atom % B.

Additional pattern
1. PDF card 9-361 [Plessey Co. Ltd., Caswell, Towcester, Northants, England].

References

Kiessling, R. (1949). Acta Chem. Scand. 3, 595.
Papesch, G., Nowotny, H., and Benesovsky, F. (1973). Monatsh. Chem. 104, 933.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±6	hkℓ	2θ(°)
3.936	5	0 2 0	22.57
2.776	38	1 1 0	32.22
2.351	74	0 2 1	38.25
2.016	100	1 1 1	44.92
1.965M	79	0 4 0	46.15
1.965M		1 3 0	46.15
1.6322	32	1 3 1	56.32
1.4829	14	2 0 0	62.59
1.4663	17	0 0 2	63.38
1.3881	1L	2 2 0	67.41
1.3111	6	0 6 0	71.96
1.2961	12	1 1 2	72.93
1.2555	34	1 5 1	75.69
1.2543	30	2 2 1	75.78
1.1970	9	0 6 1	80.11
1.1840	12	2 4 0	81.17
1.1752M	30	0 4 2	81.91
1.1752M		1 3 2	81.91
1.0980	13	2 4 1	89.10
1.0509	13	1 7 0	94.27
1.0427	14	2 0 2	95.25

Chromium Chloride $CrCl_3$

Synonyms
1. Chromic chloride
2. Chromium trichloride

CAS registry no.
10025-73-7

Sample
The sample was obtained from Fisher Scientific Co., Fair Lawn, N.J.

Color
Deep purple red.

Structure
Monoclinic, A2/m (12), Z = 4, pseudo-hexagonal. The structure was determined by Morosin and Narath [1964]. This form exists at room temperature.

Lattice constants of this sample

a = 6.123(2) Å
b = 10.311(3)
c = 5.956(5)
β = 108.64(5)°

a/b = 0.5938
c/b = 0.5776

Volume
356.3 $Å^3$

Density
(calculated) 2.952 g/cm^3

Figures of merit
F_{19} = 13.2 (0.018,80)
M_{19} = 16.0

Reference intensity
$I/I_{corundum}$ = 4.5(2)

Polymorphism
There is a hexagonal form found by Wooster [1930] and a low temperature form also found by Morosin and Narath [1964].

Additional pattern
1. PDF card 6-535 [Handy and Gregory, 1952]

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.80	100	1 0 0	15.27
5.154	1	0 2 0	17.19
3.849	1L	1 2 0	23.09
2.936M	2	0 3 1	30.42
2.936M		-1 0 2	30.42
2.901	14	2 0 0	30.80
2.816	1	0 0 2	31.75
2.577	1	0 4 0	34.78
2.475	2	0 2 2	36.27
2.460	6	1 3 1	36.49
1.934	1	3 0 0	46.94
1.911	1	2 3 1	47.54
1.754	3	-3 3 1	52.09
1.720	3	-1 3 3	53.21
1.6511M	1	3 1 1	55.62
1.6511M		0 3 3	55.62
1.6478M	1	1 6 0	55.74
1.5039	1L	3 3 1	61.62
1.4498M	6	-3 5 1	64.19
1.4498M		4 0 0	64.19
1.4115M	1	0 0 4	66.15
1.4115M		-2 2 4	66.15
1.3954M	1	4 2 0	67.01
1.3954M		-4 3 1	67.01

References

Handy, L. L. and Gregory, N. W. (1952). J. Am. Chem. Soc. 74, 891.
Morosin, B. and Narath, A. (1964). J. Chem. Phys. 40, 1958.
Wooster, N. (1930). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 74, 363.

Chromium Iron Oxide, $Cr_{1.3}Fe_{0.7}O_3$

Sample
The sample was obtained from the City Chemical Corp., New York, N. Y. It was labelled iron chromite ($FeCr_2O_4$). The approximate composition was determined by the relation of the cell parameters to those of Fe_2O_3 and Cr_2O_3. This is a solid solution between hematite (Fe_2O_3) and chromic oxide (Cr_2O_3).

Color
Dark brown

Structure
Hexagonal, $R\bar{3}c$ (167), Z = 6. The structure of Cr_2O_3 was determined by Wretblad [1930]. The structure of hematite (Fe_2O_3) was determined by Davey [1923].

Lattice constants of this sample

a = 4.9965(6) Å
c = 13.621(3)

c/a = 2.7261

Volume
294.49 Å^3

Density
(calculated) 5.233 g/cm^3

Figure of merit
F_{20} = 51.0(0.014,29)

Reference intensity
$I/I_{corundum}$ = 2.11(8)

References
Davey, W. P. (1923). Phys. Rev. 21, 716.
Wretblad, P. E. (1930). Z. Anorg. Chem. 189, 329.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
3.654	43	0 1 2	24.34
2.676	100	1 0 4	33.46
2.499	73	1 1 0	35.90
2.270	4	0 0 6	39.67
2.189	27	1 1 3	41.21
2.063	4	2 0 2	43.85
1.8268	33	0 2 4	49.88
1.6801	66	1 1 6	54.58
1.5896	5	1 2 2	57.97
1.5849	6	0 1 8	58.16
1.4738	23	2 1 4	63.02
1.4421	25	3 0 0	64.57
1.3380	1	2 0 8	70.30
1.2988	12	1 0 10	72.75
1.2488	6	2 2 0	76.17
1.2179	3	3 0 6	78.47
1.1794	2	1 2 8	81.56
1.1528	4	0 2 10	83.86
1.1319	7	1 3 4	85.77
1.0945	7	2 2 6	89.46

Synonyms
1. Chromic acid anhydride
2. Chromium trioxide

CAS registry no.
1333-82-0

Sample
The sample was from J. T. Baker Chemical Co., Phillipsburg, NJ.

Color
Dark reddish brown.

Structure
Orthorhombic, Ama2 (40), Z = 4. The structure of CrO_3 was studied by Bräkken [1931] and refined by Byström and Wilhelmi [1950].

Lattice constants of this sample

a = 5.7494(15) Å
b = 8.556(2)
c = 4.7961(11)

a/b = 0.6720
c/b = 0.5606

Volume
235.93 $Å^3$

Density
(calculated) 2.815 g/cm^3

Figure of merit
F_{30} = 56.8(0.016,32)

Reference intensity
$I/I_{corundum}$ = 1.41(13)

Additional pattern
1. PDF card 9-47 [Byström and Wilhelmi, 1950]

References
Bräkken, H. (1931). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 78, 484.
Byström, A. and Wilhelmi, K.-A. (1950). Acta Chem. Scand., 4, 1131.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
4.279	19	0 2 0	20.74
4.186	90	0 1 1	21.21
3.435	100	1 2 0	25.92
3.383	64	1 1 1	26.32
2.874	44	2 0 0	31.09
2.454	4	0 3 1	36.59
2.398	17	0 0 2	37.48
2.370	18	2 1 1	37.94
2.255	18	1 3 1	39.94
2.139	2	0 4 0	42.21
2.091	2	0 2 2	43.23
2.006	8	1 4 0	45.17
1.966	10	1 2 2	46.14
1.866	2	2 3 1	48.77
1.842	5	2 0 2	49.43
1.749	10	3 2 0	52.26
1.743	11	3 1 1	52.44
1.7168	5	2 4 0	53.32
1.6921	3	2 2 2	54.16
1.6112	3	0 5 1	57.12
1.5954	2	0 4 2	57.74
1.5706	3	0 1 3	58.74
1.5512	1	1 5 1	59.55
1.5380	2	1 4 2	60.11
1.5159	4	1 1 3	61.08
1.5097	4	3 3 1	61.36
1.4366	6	4 0 0	64.85
1.4262	3	0 6 0	65.38
1.4124	4	3 2 2	66.10
1.4062	6	2 5 1	66.43
1.3956	3	2 4 2	67.00
1.3795	5	2 1 3	67.89
1.3555	6	1 3 3	69.26
1.2773	2	2 6 0	74.18

Cinchonine, $C_{19}H_{22}N_2O$

Synonym
1. (9S)-Cinchonan-9-oℓ

CAS registry no.
118-10-5

Sample
The sample was obtained from the Eastman Kodak Co., Rochester, N. Y. It was recrystallized from ethanol.

Color
Colorless

Structure
Monoclinic, $P2_1/*$, Z = 2. The unit cell and space group were determined by Paretzkin [1956].

Lattice constants of this sample

a = 11.091(2) Å
b = 7.200(3)
c = 10.774(2)
β = 107.95(2)°

a/b = 1.5404
c/b = 1.4964

Volume
818.48 $Å^3$

Density
(calculated) 1.195 g/cm^3

Figure of merit
F_{30} = 46.6(0.012,52)

Additional pattern
1. PDF card 7-526 [Paretzkin, Polytechnic Institute of Brooklyn].

References
Paretzkin, B. (1956). Acta Crystallogr. 9, 290.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
10.53	100	1 0 0	8.39
8.84	1L	-1 0 1	10.00
6.43	2	1 0 1	13.76
5.898	10	0 1 1	15.01
5.583	1	-1 1 1	15.86
5.417	4	-2 0 1	16.35
5.301	20	-1 0 2	16.71
5.282	24	2 0 0	16.77
5.119	19	0 0 2	17.31
4.795	4	1 1 1	18.49
4.423	3	-2 0 2	20.06
4.327	5	-2 1 1	20.51
4.251	7	2 1 0	20.88
4.197	21	2 0 1	21.15
4.135	10	1 0 2	21.47
3.770	2	-2 1 2	23.58
3.623	10	2 1 1	24.55
3.586M	3	-1 0 3	24.81
3.586M		1 1 2	24.81
3.437	1L	-3 0 2	25.90
3.409	1L	1 2 0	26.12
3.288	1L	-3 1 1	27.10
3.213M	1	2 0 2	27.74
3.213M		-1 1 3	27.74
3.161	1	3 1 0	28.21
3.102	1	-3 1 2	28.76
3.089	1	0 1 3	28.88
3.049	1L	3 0 1	29.27
2.936	2	2 1 2	30.42
2.809	2	3 1 1	31.83
2.770	1L	-4 0 1	32.29
2.761	1L	1 1 3	32.40
2.726	1L	-3 1 3	32.83
2.708	1L	-4 0 2	33.05
2.687	1	-1 0 4	33.32
2.638	1L	4 0 0	33.96
2.556	1	3 0 2	35.08
2.541	1	-1 2 3	35.29
2.534M	1	-4 1 2	35.39
2.534M		2 0 3	35.39
2.480	1L	0 2 3	36.19
2.464M	1L	-2 2 3	36.43
2.464M		-3 0 4	36.43
2.408	1	3 1 2	37.31
2.388	1L	2 1 3	37.63

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
2.328	1L	3 2 1	38.64
2.279	1L	-3 2 3	39.51
2.263	1L	4 1 1	39.81
2.218	1L	1 1 4	40.65
2.208	1L	-4 0 4	40.83
2.165	1L	-4 2 2	41.69
2.140	1L	-1 0 5	42.19
2.111+	1	5 0 0	42.80
2.111+		-5 0 3	42.80
2.082	1L	2 3 1	43.43
2.069M	1L	-3 0 5	43.72
2.069M		2 0 4	43.72
2.051+	1L	-1 1 5	44.12
2.051+		0 0 5	44.12
2.024M	1L	5 1 0	44.74
2.024M		-5 1 3	44.74
2.012M	1L	4 1 2	45.02
2.012M		-3 3 1	45.02
1.9898	1L	-3 1 5	45.55
1.9570M	1L	-2 3 3	46.36
1.9570M		1 2 4	46.36
1.9514M	1L	5 0 1	46.50
1.9514M		-5 0 4	46.50
1.8846M	1L	5 1 1	48.25
1.8846M		-4 2 4	48.25
1.8795M	1L	-5 2 1	48.39
1.8795M		-5 2 2	48.39
1.8389	1L	-1 2 5	49.53
1.8115	1L	4 2 2	50.33
1.8065	1L	-6 0 3	50.48
1.7932	1L	2 2 4	50.88

Synonym
1. 4-[3-(2-Chlorothioxanthen-9-ylidene)propyl] -1-piperazineethanol dihydrate

Sample
The sample was supplied by J. Rodgers, University of Adelaide, Adelaide, South Australia. Chemical analysis gave weight percents indicating that the dihydrate is the most probable formula.

Color
Colorless

Structure
Triclinic, P*, Z = 2. The unit cell was measured on a single crystal diffractometer by V. Himes at NBS (priv. comm.). The value of Z was assumed from the measured density.

Lattice constants of this sample

a = 7.773(3) Å
b = 21.939(11)
c = 6.518(4)
α = 91.60(5)°
β = 93.06(4)
γ = 90.06(4)

a/b = 0.3543
c/b = 0.2971

Volume
1110. $Å^3$

Density
(calculated) 1.308 g/cm^3
(measured) 1.34 g/cm^3

Figure of merit
F_{30} = 23.0(0.016,80)

Reference intensity
$I/I_{corundum}$ = 1.01(5)

Polymorphism
The form described here is the inactive isomer having no neuroleptic activity. An active isomer also exists.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} σ = ±6	hkℓ	2θ(°)
22.02	100	0 1 0	4.01
11.00	15	0 2 0	8.03
7.32+	38	-1 1 0	12.08
7.32+		1 1 0	12.08
6.29	39	0 -1 1	14.07
5.65	11	0 -2 1	15.66
5.48	4	0 4 0	16.15
5.34	16	-1 3 0	16.59
5.122	7	-1 0 1	17.30
5.012	13	-1 -1 1	17.68
4.792	43	0 3 1	18.50
4.721	33	1 1 1	18.78
4.609	55	-1 2 1	19.24
4.405	3	1 2 1	20.14
4.243	12	-1 -3 1	20.92
4.135	4	0 4 1	21.47
3.882	20	2 0 0	22.89
3.824+	18	-2 1 0	23.24
3.824+		-1 5 0	23.24
3.703	12	-1 4 1	24.01
3.658+	45	-2 2 0	24.31
3.658+		2 2 0	24.31
3.597	7	1 4 1	24.73
3.431	32	-2 3 0	25.95
3.371M	44	-2 1 1	26.42
3.371M		-1 -5 1	26.42
3.294	17	1 -5 1	27.05
3.269	21	-2 -2 1	27.26
3.248M	19	0 0 2	27.44
3.248M		-2 2 1	27.44
3.221M	15	0 -6 1	27.67
3.221M		1 5 1	27.67
3.167M	11	-2 4 0	28.15
3.167M		2 4 0	28.15
3.136M	10	2 -2 1	28.44
3.136M		0 7 0	28.44
3.094	4	0 2 2	28.83
2.993	8	2 -3 1	29.83
2.960	6	2 3 1	30.17
2.941M	5	1 0 2	30.37
2.941M		0 3 2	30.37
2.795M	4	-1 3 2	32.00
2.795M		0 7 1	32.00
2.780	3	2 4 1	32.17
2.740	1	0 8 0	32.66

d(Å)	I^{rel} $\sigma = \pm 6$	hkℓ	2θ(°)
2.678	6	-2 5 1	33.43
2.643	3	-1 4 2	33.89
2.516	1	3 2 0	35.66
2.449M	1	2 -6 1	36.66
2.449M		-3 0 1	36.66
2.440+	1	-3 3 0	36.81
2.440+		-2 7 0	36.81
2.317M	5	-1 6 2	38.84
2.317M		-3 3 1	38.84
2.299M	5	-2 4 2	39.15
2.299M		3 2 1	39.15
2.237	4	2 8 0	40.29

Synonym
1. Copper phosphate hydrate

CAS registry no.
1318-84-9

Sample
The sample was prepared at NBS by D. Misra by reaction of hydroxyapatite with $Cu(NO_3)_2$ solution. The material was dried at 55 °C.

Color
Light yellow green

Structure
Orthorhombic, Pnnm (58), Z = 4. The lattice constants of libethenite were determined by Strunz [1936]. The structure was determined by Heritsch [1940].

Lattice constants of this sample

a = 8.0678(10) Å
b = 8.4100(15)
c = 5.8896(7)

a/b = 0.9593
c/b = 0.7003

Volume
399.61 $Å^3$

Density
(calculated) 3.974 g/cm^3

Figure of merit
F_{30} = 53.6(0.012,45)

Reference intensity
$I/I_{corundum}$ = 1.13(4)

Additional patterns
1. PDF card 8-107 [Strunz, 1936]
2. PPF card 1-274 [Hanawalt et al., 1938]

References

Henawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Heritsch, H. (1940). Z. Kristallogr. Kristallogeometrie Kristallphys. Kristallchem. 102, 1.
Strunz, H. (1936). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 94, 63.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.813	93	1 1 0	15.23
4.818	100	0 1 1	18.40
4.751	68	1 0 1	18.66
4.137	6	1 1 1	21.46
3.729	42	1 2 0	23.84
3.638	15	2 1 0	24.45
2.946	18	0 0 2	30.32
2.912	72	2 2 0	30.68
2.647	43	1 3 0	33.84
2.627	61	1 1 2	34.10
2.610	19	2 2 1	34.33
2.561	25	3 1 0	35.01
2.532	10	0 3 1	35.43
2.446	11	3 0 1	36.71
2.414M	26	1 3 1	37.21
2.414M		0 2 2	37.21
2.377	21	2 0 2	37.81
2.348	10	3 1 1	38.30
2.312	21	1 2 2	38.93
2.288	4	2 1 2	39.34
2.265	3	3 2 0	39.77
2.071	6	2 2 2	43.67
2.017	1	4 0 0	44.91
1.9682	3	1 3 2	46.08
1.9411	3	3 3 0	46.76
1.9326	6	3 1 2	46.98
1.9237	6	1 4 1	47.21
1.9077	5	1 0 3	47.63
1.8607M	5	4 1 1	48.91
1.8607M		1 1 3	48.91
1.8196	2	4 2 0	50.09
1.8139	2	2 3 2	50.26
1.7955	2	3 2 2	50.81
1.7370M	2	4 2 1	52.65
1.7370M		1 2 3	52.65
1.7111	11	0 4 2	53.51
1.6643	7	4 0 2	55.14
1.6462	3	1 5 0	55.80
1.6330	2	4 1 2	56.29
1.6277	3	2 2 3	56.49
1.6201	10	3 3 2	56.78
1.5951	4	3 4 1	57.75
1.5849+	9	3 0 3	58.16
1.5849+		5 1 0	58.16
1.5767M	7	4 3 1	58.49

d(Å)	I^{rel} $\sigma = \pm3$	hkℓ	2θ(°)
1.5767M		1 3 3	58.49
1.5590	4	3 1 3	59.22
1.5472	9	4 2 2	59.72
1.5302	3	5 1 1	60.45
1.5063	3	5 2 0	61.51
1.4724	7	0 0 4	63.09
1.4554	6	4 4 0	63.91
1.4276	3	1 1 4	65.31

β-L-Glutamic Acid, $C_5H_9NO_4$

Synonyms
1. β-L-glutaminic acid
2. β-L-2-aminopentanedioic acid

CAS registry no.
56-86-0

Sample
The sample was obtained from Sigma Chemical Co., St. Louis, MO.

Color
Colorless

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 8. The structure was determined by Hirokawa [1955].

Lattice constants of this sample

a = 6.9651(15) Å
b = 17.308(3)
c = 5.1690(14)

a/b = 0.4024
c/b = 0.2986

Volume
623.12 $Å^3$

Density
(calculated) 1.568 g/cm^3

Figure of merit
F_{30} = 48.3(0.016,39)

Reference intensity
$I/I_{corundum}$ = 0.65(3)

Polymorphism
There is also an orthorhombic α-form found by Bernal [1931].

References

Bernal, J. D. (1931). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 78, 363.
Hirokawa, S. (1955). Acta Crystallogr. 8, 637.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
8.65	34	0 2 0	10.22
6.46	10	1 1 0	13.69
4.960	9	0 1 1	17.87
4.445M	28	1 3 0	19.96
4.445M		0 2 1	19.96
4.323	40	0 4 0	20.53
4.155	100	1 0 1	21.37
4.042	75	1 1 1	21.97
3.854	13	0 3 1	23.06
3.746	24	1 2 1	23.73
3.678	10	1 4 0	24.18
3.482	64	2 0 0	25.56
3.415	43	2 1 0	26.07
3.372	6	1 3 1	26.41
3.320	3	0 4 1	26.83
3.232	18	2 2 0	27.58
3.101	10	1 5 0	28.77
2.983	26	2 3 0	29.93
2.887M	70	2 0 1	30.95
2.887M		0 6 0	30.95
2.849	12	2 1 1	31.37
2.741	6	2 2 1	32.64
2.712	12	2 4 0	33.00
2.664	31	1 6 0	33.62
2.583M	12	0 0 2	34.70
2.583M		2 3 1	34.70
2.520	29	0 6 1	35.60
2.475	8	0 2 2	36.27
2.455	4	2 5 0	36.57
2.402	3	2 4 1	37.41
2.398	3	1 1 2	37.47
2.367	12	1 6 1	37.99
2.358	5	0 3 2	38.13
2.330	8	1 7 0	38.61
2.303	2	3 1 0	39.09
2.231	14	0 7 1	40.39
2.154	5	3 3 0	41.91
2.125	6	1 7 1	42.50
2.102	8	3 1 1	42.99
2.057	6	3 2 1	43.98

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
2.040	8	2 6 1	44.38
2.017M	8	2 2 2	44.91
2.017M		2 7 0	44.91
1.995	3	0 8 1	45.43
1.988	4	3 3 1	45.59
1.953	2	2 3 2	46.47
1.924	3	0 6 2	47.19
1.919	3	1 8 1	47.32
1.902	4	3 4 1	47.79
1.878	4	2 7 1	48.44
1.855M	5	1 6 2	49.07
1.855M		1 9 0	49.07
1.838	1	2 8 0	49.55
1.806	1	3 5 1	50.50
1.803	1	0 9 1	50.59
1.744	3	1 9 1	52.42
1.733	3	4 1 0	52.77
1.729	5	1 7 2	52.90
1.718	4	3 1 2	53.28
1.706M	3	3 6 1	53.68
1.706M		4 2 0	53.68
1.6921	2	3 7 0	54.16
1.6838M	3	2 6 2	54.45
1.6838M		2 9 0	54.45
1.6640	3	1 1 3	55.15
1.6588	3	0 8 2	55.34
1.6505M	3	0 3 3	55.64
1.6505M		4 0 1	55.64
1.6421+	4	4 1 1	55.95
1.6421+		1 2 3	55.95
1.5982	3	1 10 1	57.63
1.5864	2	4 3 1	58.10
1.5425M	2	0 9 2	59.92
1.5425M		0 5 3	59.92
1.5211	2	2 2 3	60.85
1.5055M	1	1 5 3	61.55
1.5055M		0 11 1	61.55

Glycine, α-$C_2H_5NO_2$

Synonym
1. α-Aminoacetic acid

CAS registry no.
56-40-6

Sample
The sample from Fisher Scientific Co., Fair Lawn, NJ. was recrystallized from a mixture of water and methanol to which a small amount of ether was added.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was determined by Albrecht and Corey [1939] and refined by Marsh [1957].

Lattice constants of this sample

a = 5.4621(12) Å
b = 11.966(3)
c = 5.1077(11)
β = 111.72(2)°

a/b = 0.4565
c/b = 0.4269

Volume
310.14 $Å^3$

Density
(calculated) -.608 g/cm^3

Figure of merit
F_{30} = 40.5 (0.014,51)

Reference intensity
$I/I_{corundum}$ = 4.6(3)

Polymorphism
α-glycine, the most stable form, is obtained from water at room temperature and below, while β- and γ-glycine are obtained (together with α-glycine) from mixtures of water with acetic acid at higher temperatures [Hubig, 1958].

Additional pattern
1. PDF card 7-718 [Hanawalt et al., 1938]

References

Albrecht, G. and Corey, R. B. (1939). J. Am. Chem. Soc. 61, 1087.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Hubig, W. Z. (1958). Z. Naturforsch. B13, 633.
Marsh, R. E. (1957). Acta Crystallogr. 10, 814.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
5.98	9	0 2 0	14.80
4.670	9	1 1 0	18.99
4.410	4	0 1 1	20.12
3.874	1L	1 2 0	22.94
3.719	15	0 2 1	23.91
3.523	1L	-1 2 1	25.26
3.134	6	1 3 0	28.46
3.053	10	0 3 1	29.23
2.990	100	0 4 0	29.86
2.874	1	1 1 1	31.09
2.654	1L	1 2 1	33.75
2.532	7	0 4 1	35.42
2.481	2	2 1 0	36.18
2.453	4	-2 2 1	36.60
2.374	1L	0 0 2	37.87
2.336	1	2 2 0	38.50
2.327	1	0 1 2	38.67
2.229	1L	-2 3 1	40.43
2.205	1	0 2 2	40.90
2.166	1	1 5 0	41.67
2.143M	1	-1 3 2	42.14
2.143M		2 3 0	42.14
2.105	1	1 4 1	42.94
2.051	1L	-2 2 2	44.13
2.039	1	0 3 2	44.40
2.000	1	-2 4 1	45.30
1.994	1	0 6 0	45.46
1.935M	1	-1 4 2	46.91
1.935M		2 4 0	46.91
1.915	1	-2 3 2	47.44
1.874	1L	1 1 2	48.54
1.859M	1L	2 2 1	48.97
1.859M		0 4 2	48.97
1.839	1L	0 6 1	49.54
1.808	1L	1 2 2	50.43
1.7998	1L	-3 1 1	50.68
1.7886	1L	-2 5 1	51.02
1.7566	1L	2 3 1	52.02
1.7422M	1L	-1 5 2	52.48
1.7422M		-3 2 1	52.48
1.7129	1L	1 3 2	53.45
1.6988	1L	-1 0 3	53.93
1.6821	1L	-1 1 3	54.51
1.6557	1L	-3 3 1	55.45

Guanidinium Chloride, $CH_5N_3 \cdot HCl$

Synonym
1. Guanidine Hydrochloride

CAS registry no.
50-01-1

Sample
The sample was obtained from Mallinckrodt Chemical Works, St. Louis, MO.

Color
Colorless

Structure
Orthorhombic, Pbca(61), Z = 8. The structure was determined by Haas et al. [1965].

Lattice constants of this sample

a = 9.192(2) Å
b = 13.037(4)
c = 7.774(2)

a/b = 0.7051
c/b = 0.5963

Volume
963.6 $Å^3$

Density
(calculated) 1.362 g/cm^3

Figure of merit
F_{30} = 36.0(0.015,55)

Reference intensity
$I/I_{corundum}$ = 0.77(2)

Additional pattern
1. PDF card 3-387 [Theilacker, 1931].

References

Haas, D. J., Harris, D. R., and Mills, H. H. (1965). Acta Crystallogr. 19, 309.
Theilacker, W. (1931). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 76, 203.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
4.996	3	0 2 1	17.74
4.591	13	2 0 0	19.32
4.386	88	1 2 1	20.23
4.329	16	2 1 0	20.50
3.884	9	0 0 2	22.88
3.787	46	2 1 1	23.47
3.583	50	1 0 2	24.83
3.448	96	1 1 2	25.82
3.381	54	2 2 1	26.34
3.258	29	0 4 0	27.35
2.968	100	2 0 2	30.08
2.927	12	2 3 1	30.52
2.894	5	2 1 2	30.87
2.783	31	3 1 1	32.14
2.763	41	1 3 2	32.38
2.659	75	2 4 0	33.68
2.497	35	0 4 2	35.93
2.449M	10	2 3 2	36.66
2.449M		1 1 3	36.66
2.407M	11	0 2 3	37.33
2.407M		3 0 2	37.33
2.384	6	3 3 1	37.70
2.368	2	3 1 2	37.97
2.297	13	4 0 0	39.18
2.264	5	4 1 0	39.78
2.223	2	2 1 3	40.54
2.195	9	2 4 2	41.08
2.173M	4	4 1 1	41.52
2.173M		0 6 0	41.52
2.164	4	1 3 3	41.70
2.134	3	2 2 3	42.31
2.106M	11	1 5 2	42.91
2.106M		3 3 2	42.91
2.088	9	4 2 1	43.29
2.040	4	1 6 1	44.36
2.032	1	4 3 0	44.56
1.978	3	4 0 2	45.85
1.966M	5	4 3 1	46.14
1.966M		2 6 0	46.14
1.959	7	2 5 2	46.32
1.957M	5	3 1 3	46.37
1.957M		4 1 2	46.37
1.902	6	1 0 4	47.79
1.894M	6	3 2 3	47.99
1.894M		4 2 2	47.99

Guanidinium Chloride, $CH_5N_3 \cdot HCl$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
1.881	8	1 1 4	48.35
1.8011M	5	3 3 3	50.64
1.8011M		4 3 2	50.64
1.7683	2	3 5 2	51.65
1.7422	7	1 3 4	52.48
1.7279	5	3 6 1	52.95
1.7046	5	4 1 3	53.73
1.6909M	6	3 4 3	54.20
1.6909M		4 4 2	54.20

Hexamethylenetetramine, $C_6H_{12}N_4$

Synonym
1. 1,3,5,7-tetraazatricyclo [3.3.1.$1^{3,7}$]-decane
2. Methenamine

CAS registry no.
100-97-0

Sample
The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from ethanol. There was one line at d = 3.152 with an intensity of 1 that was not accounted for.

Color
Colorless

Structure
Cubic, $I\bar{4}3m$ (217), Z = 2. The structure was determined quantitatively by Becka and Cruickshank [1963].

Lattice constant of this sample
a = 7.0287(3) Å

Volume
347.24 Å^3

Density
(calculated) 1.341 g/cm^3

Figure of merit
F_{22} = 74.3(0.010,29)

Reference intensity
$I/I_{corundum}$ = 3.84(10)

Additional pattern
1. PDF card 3-135 [Dow Chemical Co., Midland, MI]

Reference
Becka, L. N. and Cruickshank, D. W. J. (1963). Proc. Roy. Soc. Ser. A 273, 435.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
4.968	100	1 1 0	17.84
3.517	4	2 0 0	25.30
2.870	14	2 1 1	31.14
2.485	2	2 2 0	36.12
2.224	1L	3 1 0	40.53
2.0291	6	2 2 2	44.62
1.8784	4	3 2 1	48.42
1.6560	1L	4 1 1	55.44
1.5713	1L	4 2 0	58.71
1.4984	1	3 3 2	61.87
1.4346	1L	4 2 2	64.95
1.3786	1	5 1 0	67.94
1.2832	1L	5 2 1	73.78
1.2424	1	4 4 0	76.63
1.2057	1L	5 3 0	79.42
1.1715	1L	6 0 0	82.22
1.1404	1L	6 1 1	84.98
1.0845	1L	5 4 1	90.52
1.0595	1L	6 2 2	93.28
1.0362	1L	6 3 1	96.04
.9565	1L	7 2 1	107.29
.8927	1L	7 3 2	119.29

Synonyms
1. Hydrazine sulfate
2. Hydrazonium sulfate

CAS registry no.
10034-93-2

Sample
Hydrazinium sulfate was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was recrystallized from water. The x-ray pattern was run in a humid atmosphere.

Color
Colorless

Structure
Orthorhombic, $P2_12_12_1$ (19), Z = 4. The structure was determined by Nitta et al. [1951] and refined by Jönsson and Hamilton [1970].

Lattice constants of this sample

a = 8.2579(14) Å
b = 9.178(2)
c = 5.5386(11)

a/b = 0.8997
c/b = 0.6035

Volume
419.78 $Å^3$

Density
(calculated) 2.059 g/cm^3

Figure of merit
F_{30} = 57.4 (0.013,41)

Reference intensity
$I/I_{corundum}$ = 1.47(8)

Additional pattern
1. PDF card 4-375 (Inst. of Physics, Univ. College, Cardiff, Wales)

References
Jönsson, P. G. and Hamilton, W. C. (1970). Acta Crystallogr. B26, 536.
Nitta, I., Sakurai, K., and Tomiie, Y. (1951). Acta Crystallogr. 4, 289.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} $\sigma = \pm 5$	hkℓ	1θ(°)
6.15	10	1 1 0	14.39
4.602	46	1 0 1	19.27
4.130	100	2 0 0	21.50
4.015	20	1 2 0	22.12
3.768	10	2 1 0	23.59
3.534	62	0 2 1	25.18
3.312	1	2 0 1	26.90
3.250	47	1 2 1	27.42
3.116	43	2 1 1	28.62
3.071	19	2 2 0	29.05
2.769	12	0 0 2	32.30
2.685	17	2 2 1	33.34
2.650	6	0 1 2	33.80
2.636	8	3 1 0	33.98
2.625	9	1 0 2	34.13
2.546	4	1 3 1	35.22
2.525	10	1 1 2	35.53
2.458	6	2 3 0	36.53
2.381	7	3 1 1	37.75
2.361	4	3 2 0	38.09
2.295	3	0 4 0	39.22
2.280	4	1 2 2	39.50
2.246	2	2 3 1	40.11
2.232	9	2 1 2	40.38
2.211	13	1 4 0	40.78
2.172	3	3 2 1	41.54
2.119	1	0 4 1	42.63
2.052M	2	1 4 1	44.09
2.052M		0 3 2	44.09
2.047	2	3 3 0	44.20
2.013	4	4 1 0	44.99
1.993	1	1 3 2	45.47
1.953	2	3 0 2	46.46
1.9100	14	3 1 2	47.57
1.8924	3	4 1 1	48.04
1.8850	6	2 4 1	48.24
1.8382	2	2 3 2	49.55
1.7955	1	3 2 2	50.81
1.7916	1	1 5 0	50.93
1.7824	2	4 2 1	51.21
1.7676M	5	1 1 3	51.67
1.7676M		0 4 2	51.67
1.7622	7	3 4 0	51.84
1.7114	2	4 3 0	53.50
1.6849	2	2 0 3	54.41

$d(\mathring{A})$	I^{rel} $\sigma = \pm 5$	hkℓ	2θ(°)
1.6778M	2	2 5 0	54.66
1.6778M		1 2 3	54.66
1.6579	3	2 1 3	55.37
1.6451	1	3 3 2	55.84
1.6346	3	4 3 1	56.23
1.5821M	2	5 0 1	58.27
1.5821M		2 2 3	58.27
1.5595	3	5 1 1	59.20

Iron Chloride Hydrate (Hydromolysite), $FeCl_3 \cdot 6H_2O$

Synonym
1. Ferric chloride hexahydrate

CAS registry no.
10025-77-1

Sample
The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was somewhat hygroscopic.

Color
Deep orange yellow

Structure
Monoclinic, C2/m (12), Z = 2. The structure of $FeCl_3 \cdot 6H_2O$ was determined by Lind [1961].

Lattice constants of this sample

a = 11.834(3) Å
b = 7.029(2)
c = 5.9524(13)
β = 100.47(2)°

a/b = 1.6836
c/b = 0.8468

Volume
486.8 $Å^3$

Density
(calculated) 1.844 g/cm^3

Figure of merit
F_{30} = 41.4(0.015,47)

Additional pattern
1. PDF card 1-153 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Lind, M. D. (1967). J. Chem. Phys. 47, 990.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.03	14	1 1 0	14.69
5.866	82	0 0 1	15.09
5.824	100	2 0 0	15.20
4.565	3	-2 0 1	19.43
4.412	5	-1 1 1	20.11
4.015	4	1 1 1	22.12
3.516	4	0 2 0	25.31
3.163	15	-3 1 1	28.19
3.015	2	0 2 1	29.61
2.927	3	0 0 2	30.52
2.909	5	4 0 0	30.71
2.818	2	-4 0 1	31.73
2.782	4	-2 2 1	32.15
2.754	7	3 1 1	32.49
2.736	3	-1 1 2	32.70
2.580	5	2 2 1	34.74
2.540	3	1 1 2	35.31
2.442	13	2 0 2	36.77
2.280	1L	-4 0 2	39.50
2.242	1	4 2 0	40.19
2.203	3	-2 2 2	40.93
2.199	4	-4 2 1	41.02
2.165	1	-1 3 1	41.69
2.060	2	3 1 2	43.92
2.004M	2	2 2 2	45.20
2.004M		3 3 0	45.20
2.001	2	4 2 1	45.28
1.958	5	5 1 1	46.33
1.954	5	-3 3 1	46.44
1.939	3	6 0 0	46.81
1.9096	3	-1 1 3	47.58
1.8979	4	4 0 2	47.89
1.8445	1L	3 3 1	49.37
1.8065	3	1 1 3	50.48
1.7721	2	-6 0 2	51.53
1.7559	1	2 0 3	52.04
1.7117	1L	-2 2 3	53.49
1.7058M	1	0 2 3	53.69
1.7058M		-6 2 1	53.69
1.6982	3	6 2 0	53.95
1.6815	1L	2 4 0	54.53
1.6702	1	4 2 2	54.93

Iron Fluoride Hydrate, β-$FeF_3 \cdot 3H_2O$

Synonym
1. Ferric trifluoride trihydrate

Sample
The sample was obtained from City Chemical Corp., New York, NY.

Color
Blue gray.

Structure
Tetragonal, P4/n (85), Z = 2. The structure was determined by Teufer [1964].

Lattice constants of this sample

a = 7.8326(5) Å
c = 3.8773(3)

c/a = 0.4950

Volume
237.87 $Å^3$

Density
(calculated) 2.330 g/cm^3

Figure of merit
F_{30} = 80.9(0.010,36)

Reference intensity
$I/I_{corundum}$ = 2.00(4)

Polymorphism
Nielsen [1940] reported another form of $FeF_3 \cdot 3H_2O$ which was colorless and was made by crystallization at a lower temperature than the form studied here.

Additional pattern
1. PDF card 1-202 [Hanawalt et al., 1938]

References
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Nielsen, A. H. (1940). Z. Anorg. Allgem. Chem., 244, 85.
Teufer, G. (1964). Acta Crystallogr. 17, 1480.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
5.542	100	1 1 0	15.98
3.917	54	2 0 0	22.68
3.879	14	0 0 1	22.91
3.476	49	1 0 1	25.61
3.177	25	1 1 1	28.06
2.769	28	2 2 0	32.30
2.600	10	2 1 1	34.47
2.475	31	3 1 0	36.27
2.253	1	2 2 1	39.99
2.1662	1L	3 0 1	41.66
2.0861	14	3 1 1	43.34
1.9586	11	4 0 0	46.32
1.8950	13	3 2 1	47.97
1.8817	24	1 0 2	48.33
1.8466	6	3 3 0	49.31
1.8295	3	1 1 2	49.80
1.7512	26	4 2 0	52.19
1.7061	8	4 1 1	53.68
1.6961	9	2 1 2	54.02
1.6674	3	3 3 1	55.03
1.5962	3	4 2 1	57.71
1.5569	2	3 0 2	59.31
1.5357	5	5 1 0	60.21
1.5268	2	3 1 2	60.60
1.4524	3	4 3 1	64.06
1.4468	9	3 2 2	64.34
1.4280	3	5 1 1	65.29
1.3849	1	4 4 0	67.59
1.3620	4	5 2 1	68.88
1.3570	8	4 1 2	69.17
1.3430	2	5 3 0	70.00
1.3370	1	3 3 2	70.36
1.2920	1	0 0 3	73.20
1.2691	1	5 3 1	74.74
1.2586	1L	1 1 3	75.47
1.2385	3	6 2 0	76.92
1.2275	1L	2 0 3	77.74
1.2220	1	6 1 1	78.15
1.2185	4	4 3 2	78.42
1.2036	2	5 1 2	79.58
1.1712	1	2 2 3	82.25
1.1635	4	5 2 2	82.91
1.1459	1	3 1 3	84.48

Lanthanum Nickel Platinum, $LaNi_{0.25}Pt_{4.75}$

Sample
The sample was prepared at NBS by Weisman et al. [1975].

Color
Metallic gray

Structure
Hexagonal, P6/mmm (191), Z = 1. This phase has the $CaCu_5$ type structure. The structure of $CaCu_5$ was determined by Haucke [1940].

Lattice constants of this sample

a = 5.3732(5) Å
c = 4.3574(7)

c/a = 0.8110

Volume
108.95 Å

Density
(calculated) 16.465 g/cm^3

Figure of merit
F_{20} = 69.7(0.011,26)

References
Haucke, W. (1940). Z. Anorg. Allg. Chem. 244, 17.
Weisman, I. D., Bennett, L. H., McAlister, A. J., and Watson, R. E. (1975). Phys. Rev. B 11, 82.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ	2θ(°)
4.655	36	1 0 0	19.05
3.182	10	1 0 1	28.02
2.685	18	1 1 0	33.34
2.327	40	2 0 0	38.66
2.287	100	1 1 1	39.37
2.179	32	0 0 2	41.40
2.0532	54	2 0 1	44.07
1.9730	9	1 0 2	45.96
1.7591	5	2 1 0	51.94
1.6924	7	1 1 2	54.15
1.6312	2	2 1 1	56.36
1.5901	15	2 0 2	57.95
1.5512	4	3 0 0	59.55
1.4608	21	3 0 1	63.65
1.3687	4	2 1 2	68.50
1.3436	13	2 2 0	69.96
1.2774	8	1 1 3	74.17
1.2633	3	3 0 2	75.14
1.2323	6	2 0 3	77.38
1.1632	5	4 0 0	82.94

CAS registry no.
10031-22-8

Sample
The sample originally obtained from National Lead Co. was used. These data replace a very early pattern [Swanson and Fuyat, 1953]. The new measurements have better resolution, improved intensities, and refined lattice parameters.

Major impurities
Spectrographic analysis showed 0.001 to 0.01% iron and 0.0001 to 0.001% each Ag, Al, Cu, Mg, and Si.

Color
Colorless

Structure
Orthorhombic, Pnam (62), Z = 4, isostructural with $PbCl_2$ [Bräkken and Harang, 1928]. The structure was determined by McBride [1967].

Lattice constants of this sample
a = 8.062(1) Å
b = 9.5393(13)
c = 4.7348(6)

a/b = 0.8452
c/b = 0.4964

Volume
364.1 $Å^3$

Density
(calculated) 6.695 g/cm^3

Figure of merit
F_{30} = 78.8(0.014,38)

Reference intensity
$I/I_{corundum}$ = 1.83(11)

Additional patterns
1. PDF card 5-608 [Swanson and Fuyat, 1953]
2. Bräkken and Harang [1928]
3. Döll and Klemm [1939]
4. Hanawalt, Rinn, and Frevel [1938]

References
Bräkken, H. and Harang, L. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 68, 123.
Döll, W. and Klemm, W. (1939). Z. Anorg, Allg. Chem. 241, 239.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
McBride, H. D. (1967). Diss. Abstr. B27, 3891.
Swanson, H. E. and Fuyat, R. K. (1953). Nat. Bur. Stand. U.S. Circ. 539, 2, 47.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ	2θ(°)
6.16	3	1 1 0	14.37
4.774	30	0 2 0	18.57
4.239	19	0 1 1	20.94
4.105	56	1 2 0	21.63
4.032	31	2 0 0	22.03
3.751	73	1 1 1	23.70
3.711	8	2 1 0	23.96
3.102	50	1 2 1	28.76
3.081	55	2 2 0	28.96
3.071	56	2 0 1	29.05
2.958	23	1 3 0	30.19
2.924	100	2 1 1	30.55
2.641	90	0 3 1	33.92
2.586	10	3 1 0	34.66
2.580	9	2 2 1	34.74
2.509	8	1 3 1	35.76
2.495	15	2 3 0	35.97
2.385	28	0 4 0	37.69
2.367	45	0 0 2	37.98
2.341	38	3 2 0	38.42
2.286	14	1 4 0	39.38
2.271	42	3 1 1	39.66
2.208M	55	2 3 1	40.83
2.208M		1 1 2	40.83
2.122	5	0 2 2	42.58
2.099	4	3 2 1	43.06
2.052M	18	3 3 0	44.10
2.052M		2 4 0	44.10
2.042	12	2 0 2	44.32
2.016	8	4 0 0	44.92
1.997	2	2 1 2	45.38
1.972	4	4 1 0	45.99
1.8843M	6	2 4 1	48.26
1.8843M		3 3 1	48.26
1.8773	11	2 2 2	48.45
1.8568M	4	4 2 0	49.02
1.8568M		1 5 0	49.02
1.8554	4	4 0 1	49.06
1.8483	6	1 3 2	49.26
1.7834	7	3 4 0	51.18
1.7702	12	0 5 1	51.59
1.7459	2	3 1 2	52.36
1.7291M	14	1 5 1	52.91
1.7291M		4 2 1	52.91
1.7242	10	2 5 0	53.07
1.7185	7	2 3 2	53.26
1.7023	4	4 3 0	53.81
1.6792	9	0 4 2	54.61
1.6688	7	3 4 1	54.98
1.6652	20	3 2 2	55.11

d(Å)	I^{rel} $\sigma = \pm 4$	hkℓ	2θ(°)
1.6448	4	1 4 2	55.85
1.6017	4	4 3 1	57.49
1.5896M	7	5 1 0	57.97
1.5896M		0 6 0	57.97
1.5602	2	1 6 0	59.17
1.5564M	3	0 1 3	59.33
1.5564M		3 5 0	59.33
1.5505M	4	3 3 2	59.58
1.5505M		2 4 2	59.58
1.5390	4	4 4 0	60.07
1.5346	6	4 0 2	60.26
1.5295	7	1 1 3	60.48
1.5277	7	5 2 0	60.56
1.5146	4	4 1 2	61.14
1.5068	15	5 1 1	61.49
1.4793	20	2 6 0	62.76
1.4699	6	2 0 3	63.21
1.4608M	2	4 2 2	63.65
1.4608M		1 5 2	63.65
1.4524	6	2 1 3	64.06
1.4384	1	5 3 0	64.76
1.4247	4	3 4 2	65.46
1.4138	7	0 3 3	66.03
1.4040	2	2 2 3	66.55
1.3938	2	2 5 2	67.10
1.3818	2	4 3 2	67.76
1.3759	2	5 3 1	68.09
1.3470	5	3 1 3	69.76
1.3358	7	5 4 0	70.43
1.3337	7	2 3 3	70.56
1.3196M	5	5 1 2	71.43
1.3196M		0 6 2	71.43
1.3094	5	0 7 1	72.07

Lead Iodate, $Pb(IO_3)_2$

CAS registry no.
25659-31-8

Sample
The sample was made by adding solid I_2O_5 to an aqueous solution of $Pb(NO_3)_2$. This was digested by boiling for 1 hour and filtered. The solid was then heated at 300 °C for 2 hours and at 250 °C for 16 hours.

Color
Colorless

Structure
Orthorhombic, Pnaa (56), Z = 4 [Staritzky and Walker, 1956].

Lattice constants of this sample

a = 6.090(2) Å
b = 16.690(3)
c = 5.580(2)

a/b = 0.3649
c/b = 0.3343

Volume
567.2 $Å^3$

Density
(calculated) 6.523 g/cm^3

Figure of merit
F_{30} = 31.1(0.017,58)

Reference intensity
$I/I_{corundum}$ = 11.9(5)

Additional pattern
1. PDF card 11-85 [Staritzky and Walker, 1956]

Reference
Staritzky, E. and Walker, D. I. (1956). Anal. Chem. 28, 914.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
8.36	4	0 2 0	10.57
3.996	2	1 1 1	22.23
3.694	2	1 2 1	24.07
3.309	100	1 3 1	26.92
3.047	15	2 0 0	29.29
2.999	2	2 1 0	29.77
2.931	1	1 4 1	30.47
2.864	2	0 5 1	31.20
2.784	23	0 6 0	32.12
2.673M	1L	2 0 1	33.50
2.673M		2 3 0	33.50
2.647	1	0 2 2	33.84
2.594	4	1 5 1	34.55
2.546	1L	2 2 1	35.22
2.508	1L	1 1 2	35.77
2.462	1	2 4 0	36.47
2.307	1L	1 3 2	39.01
2.250M	1	2 5 0	40.04
2.250M		2 4 1	40.04
2.194	1L	0 7 1	41.10
2.086M	1L	0 8 0	43.34
2.086M		2 5 1	43.34
2.055	20	2 6 0	44.04
2.043	6	2 1 2	44.31
1.996	1	2 2 2	45.39
1.969	11	0 6 2	46.05
1.930	1L	2 3 2	47.05
1.895	1	3 1 1	47.98
1.877	1L	2 7 0	48.47
1.860M	3	3 2 1	48.94
1.860M		1 8 1	48.94
1.804	9	3 3 1	50.56
1.751	1	2 5 2	52.20
1.735	2	3 4 1	52.70
1.7215	1	2 8 0	53.16
1.6909	19	1 9 1	54.20
1.6707	1	0 8 2	54.91
1.6538	10	2 6 2	55.52
1.6373	1L	1 4 3	56.13
1.5691	1L	1 5 3	58.80
1.5569	1L	2 7 2	59.31
1.5460	1L	1 10 1	59.77
1.5220	1	4 0 0	60.81
1.4643+	1L	0 11 1	63.48
1.4643+		2 8 2	63.48
1.4235	1	1 11 1	65.52
1.4079	1	3 8 1	66.34
1.3905	2	0 12 0	67.28

CAS registry no.
1310-65-2

Sample
The sample was obtained from Fisher Scientific Co., Fair Lawn, N. J. It contained a small amount of $LiOH \cdot H_2O$ and was somewhat unstable in air. The d-spacing patterns were run with the sample in vacuum grease, and the intensity patterns run with the sample in Canada Balsam.

Structure
Tetragonal, P4/nmm (129), Z = 2. The structure of LiOH was determined by Ernst [1933].

Lattice constants of this sample

a = 3.5528(5) Å
c = 4.3476(9)

c/a = 1.2237

Volume
54.88 $Å^3$

Density
(calculated) 1.449 g/cm^3

Figure of merit
F_{15} = 63.5(0.013,18)

Additional pattern
1. PDF card 4-708 [Ernst, 1933]

Reference
Ernst, T. (1933). Z. Phys. Chem. Leipzig B20, 65.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
4.352	43	0 0 1	20.39
2.754	100	1 0 1	32.49
2.514	22	1 1 0	35.69
2.174M	2	1 1 1	41.51
2.174M		0 0 2	41.51
1.8540	6	1 0 2	49.10
1.7760	16	2 0 0	51.41
1.6435M	13	2 0 1	55.90
1.6435M		1 1 2	55.90
1.4919	10	2 1 1	62.17
1.4492	1	0 0 3	64.22
1.3754	1	2 0 2	68.12
1.3418	1	1 0 3	70.07
1.2828	3	2 1 2	73.81
1.2552	4	1 1 3	75.71
1.2068	1	2 2 1	79.33
1.1427	1	3 0 1	84.77

CAS registry no.
12007-62-4

Sample
The sample was prepared by heating a 1:4 molar mixture of $MgCO_3$ and H_3BO_3 at 600 °C for 3 days, followed by heating one hour at 800 °C, and 16 hours at 600 °C with intermittent grinding. There was a very small amount of $Mg_2B_2O_5$ present.

Color
Colorless

Structure
Orthorhombic, Pbca (61), Z = 8 [Kuzel, 1964]. Davis and Knight [1945] reported that this phase had the composition of MgB_2O_4.

Lattice constants of this sample

a = 8.596(2) Å
b = 13.729(4)
c = 7.956(2)

a/b = 0.6261
c/b = 0.5795

Volume
938.9 $Å^3$

Density
(calculated) 2.540 g/cm^3

Figure of merit
F_{30} = 32.8(0.014,64)

Reference intensity
$I/I_{corundum}$ = 0.57(11)

Additional pattern
1. PDF card 17-927 [Kuzel, 1964]

References
Davis, H. M. and Knight, M. A. (1945). J. Amer. Ceram. Soc. 28, 100.
Kuzel, H.-J. (1964). Neues Jahrb. Mineral. Monatsh. 1964, 357.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
6.86	21	0 2 0	12.89
5.37	19	1 1 1	16.50
5.196	98	0 2 1	17.05
4.447	81	1 2 1	19.95
4.098	24	2 1 0	21.67
3.976	100	0 0 2	22.34
3.636	37	2 2 0	24.46
3.607M	42	1 0 2	24.66
3.607M		1 3 1	24.66
3.441	64	0 2 2	25.87
3.314	5	2 2 1	26.88
3.194	9	1 2 2	27.91
3.134	34	2 3 0	28.46
2.959	13	1 4 1	30.18
2.916M	29	2 0 2	30.63
2.916M		2 3 1	30.63
2.836	51	1 3 2	31.52
2.683	33	2 4 0	33.37
2.644	8	3 1 1	33.87
2.542	6	2 4 1	35.28
2.485	18	1 5 1	36.12
2.474	21	0 2 3	36.28
2.325M	6	3 0 2	38.70
2.325M		3 3 1	38.70
2.223M	43	2 4 2	40.54
2.223M		2 5 1	40.54
2.203	11	3 2 2	40.93
2.149	10	4 0 0	42.01
2.123	2	4 1 0	42.55
2.074	3	3 3 2	43.61
2.051M	5	4 1 1	44.12
2.051M		4 2 0	44.12
2.001	8	2 5 2	45.29
1.987M	10	0 0 4	45.61
1.987M		4 2 1	45.61
1.958	7	2 6 1	46.34
1.945	16	4 3 0	46.67
1.924M	21	3 4 2	47.19
1.924M		3 5 1	47.19
1.911	7	0 2 4	47.54
1.886	4	2 4 3	48.20
1.872	4	4 1 2	48.60
1.872		3 2 3	48.60
1.861	3	1 5 3	48.89
1.822M	7	4 2 2	50.02
1.822M		4 4 0	50.02
1.789	9	2 1 4	51.02
1.7450M	5	2 2 4	52.39
1.7450M		3 6 1	52.39
1.7227	8	1 7 2	53.12

CAS registry no.
13446-17-8

Sample
The sample obtained from the Eastman Kodak Co., Rochester, NY, was recrystallized from an aqueous solution at room temperature.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), Z = 2. It was assumed to be isostructural with $Co(IO_3)_2 \cdot 4H_2O$ and β-$Ni(IO_3)_2 \cdot 4H_2O$ from a comparison of the powder patterns and the cell sizes. The latter compounds were studied by Abrahams et al. [1973]. Preliminary lattice constants for $Mg(IO_3)_2 \cdot 4H_2O$ were obtained by the use of the axial ratios given by Groth [1908].

Lattice constants of this sample

a = 8.5063(15) Å
b = 6.6362(15)
c = 8.3306(12)
β = 100.59(1)°

a/b = 1.2818
c/b = 1.2554

Volume
462.25 $Å^3$

Density
(calculated) 3.206 g/cm^3

Figure of merit
F_{30} = 47.8(0.015,41)

Reference intensity
$I/I_{corundum}$ = 2.44(8)

Additional pattern
1. PDF card 20-676 [University College, Cardiff, Wales]

References
Abrahams, S. C., Sherwood, R. C., Bernstein, J. L., and Nassau, K. (1973). J. Solid State Chem. 7, 205.
Groth, P. (1908). Chemische Krystallographie II (Engelmann, Leipzig, Germany) p. 120.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
8.18	24	0 0 1	10.81
5.154	100	0 1 1	17.19
4.631	13	-1 1 1	19.15
4.174M	74	2 0 0	21.27
4.174M		1 1 1	21.27
4.094	12	0 0 2	21.69
3.535	8	2 1 0	25.17
3.478	55	2 0 1	25.59
3.445	48	-2 1 1	25.84
3.413	8	-1 1 2	26.09
3.318	5	0 2 0	26.85
3.236	13	-2 0 2	27.54
3.077M	15	2 1 1	29.00
3.077M		0 2 1	29.00
3.052	2	1 1 2	29.24
2.954	30	-1 2 1	30.23
2.912	4	-2 1 2	30.68
2.826	4	1 2 1	31.64
2.728	22	0 0 3	32.80
2.599	9	2 2 0	34.48
2.577M	6	-3 1 1	34.78
2.577M		0 2 2	34.78
2.570	6	3 1 0	34.88
2.540	9	-1 1 3	35.31
2.525	5	0 1 3	35.52
2.506	5	-2 0 3	35.81
2.493	6	2 1 2	36.00
2.397	6	2 2 1	37.49
2.387	11	1 2 2	37.66
2.364	3	-3 1 2	38.04
2.343M	2	-2 1 3	38.39
2.343M		3 1 1	38.39
2.316	4	-2 2 2	38.85
2.311	3	1 1 3	38.94
2.137M	17	1 3 0	42.26
2.137M		0 3 1	42.26
2.114	6	2 0 3	42.74
2.089M	4	4 0 0	43.27
2.089M		2 2 2	43.27
2.046M	4	0 0 4	44.23
2.046M		1 3 1	44.23
2.019M	11	-4 1 1	44.85
2.019M		-4 0 2	44.85
2.015	11	2 1 3	44.95
1.994	4	4 1 0	45.46
1.956M	4	0 1 4	46.39
1.956M		2 3 0	46.39
1.941M	4	4 0 1	46.76
1.941M		-2 3 1	46.76
1.904	5	-2 1 4	47.72

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2Θ(°)
1.866	1	2 3 1	48.77
1.834	3	1 1 4	49.68
1.7925	2	3 2 2	50.90
1.7619	3	-1 2 4	51.85
1.7425	2	0 2 4	52.47
1.7370	4	4 0 2	52.65
1.7327	4	3 3 0	52.79
1.7236M	7	-4 2 2	53.09
1.7236M		-1 3 3	53.09
1.6801	2	4 1 2	54.58
1.6758	2	4 2 1	54.73
1.6654	2	-3 3 2	55.10
1.6465	2	1 3 3	55.79
1.6298	1	-2 0 5	56.41
1.6190	1	-4 0 4	56.82
1.6092	2	-5 1 2	57.20
1.5901	4	0 1 5	57.95
1.5730	2	-4 1 4	58.64

CAS registry no.
7439-96-5

Sample
The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ. It was annealed in vacuum at 650 °C for 4 hours.

Color
Metallic gray

Structure

Cubic, $I\bar{4}3m$ (217), Z = 58 [Gazzara et al., 1967].

Lattice constant of this sample

a = 8.9121 (4) Å

Volume
707.85 $Å^3$

Density
(calculated) 7.475 g/cm^3

Figure of merit
F_{30} = 69.9 (0.012,37)

Polymorphism
There are also β, γ, and δ Mn, the most probable transition temperatures being α ⇄ β, 700 °C; β ⇄ γ, 1079 °C; α ⇄ δ 1143 °C [Sully, 1955].

Additional patterns
1. PDF card 1-1237 [Hanawalt et al., 1938].
2. PDF card 20-180 [Swanson et al., 1969].

References
Gazzara, C. P., Middleton, R. M., Weiss, R. J., and Hall, E. O. (1967). Acta Crystallogr. 22, 859.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Sully, A. H. (1955). Manganese (Butterworth Scientific Publications, London), p. 127.
Swanson, H. E., McMurdie, H. F., Morris, M. C., and Evans, E. H. (1969). Nat'l. Bur. Std. U.S. Monogr. 25, Sec. 7, 142.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
3.641	1L	2 1 1	24.43
3.153	1	2 2 0	28.28
2.571	3	2 2 2	34.87
2.382	3	3 2 1	37.74
2.227	7	4 0 0	40.48
2.101	100	4 1 1	43.01
1.8994	24	3 3 2	47.85
1.8193	9	4 2 2	50.10
1.7475	14	5 1 0	52.31
1.6274	1	5 2 1	56.50
1.5286	1L	5 3 0	60.52
1.4857	1	6 0 0	62.46
1.4460	1	6 1 1	64.38
1.4088	1L	6 2 0	66.29
1.3754	1L	5 4 1	68.12
1.3435	2	6 2 2	69.97
1.3138	1L	6 3 1	71.79
1.2864	4	4 4 4	73.57
1.2605	7	7 1 0	75.34
1.2125	17	7 2 1	78.88
1.1911	3	6 4 2	80.59
1.1701	2	7 3 0	82.34
1.1317	3	7 3 2	85.79
1.0969	2	8 1 1	89.22
1.0806	1	8 2 0	90.93
1.0652	1	6 5 3	92.63
1.0504	6	8 2 2	94.33
1.0361	1	8 3 1	96.05
1.0223	1L	6 6 2	97.79
1.0091	1	7 5 2	99.52

Synonym
1. Mercurous Acetate

CAS registry no.
631-60-7

Sample
$Hg_2(NO_3)_2 \cdot 2H_2O$ was dissolved in water with addition of 25% HNO_3 and treated with a solution of CH_3CO_2Na. The precipitate was washed with cold water and dried in a desiccator [Brauer, 1963].

Color
Colorless

Structure
Monoclinic, A*/*, Z = 2 [Puff et al., 1965].

Lattice constants of this sample

a = 12.185(3) Å
b = 5.966(2)
c = 5.1867(13)
β = 100.08(2)°

a/b = 2.0424
c/b = 0.8694

Volume
371.2 $Å^3$

Density
(calculated) 4.645 g/cm^3

Figure of merit
F_{30} = 54.5(0.013,42)

Additional pattern
1. PDF card 19-799 [Puff et al., 1965]

References

Brauer, G. (1963). Handbook of Preparative Inorganic Chemistry, (Academic Press, New York, NY) p. 1120.
Puff, H., Lorbacher, G., and Skrabs, R. (1965). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 122, 156.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
12.02	100	1 0 0	7.35
6.00	1	2 0 0	14.74
4.001	3	3 0 0	22.20
3.877	11	0 1 1	22.92
3.849	15	-1 1 1	23.09
3.553	2	1 1 1	25.04
3.477	14	-2 1 1	25.60
3.079	1	2 1 1	28.98
3.000	14	4 0 0	29.76
2.894	5	1 2 0	30.87
2.615	4	3 1 1	34.26
2.593	2	-1 0 2	34.57
2.544	1L	-4 1 1	35.25
2.514	3	-2 0 2	35.69
2.399	8	5 0 0	37.46
2.346	2	-3 0 2	38.33
2.233	8	4 1 1	40.35
2.215	2	2 0 2	40.71
2.174	2	-5 1 1	41.51
2.137	1	-4 0 2	42.26
2.115	3	4 2 0	42.72
2.000M	6	6 0 0	45.30
2.000M		3 0 2	45.30
1.956	1	-1 2 2	46.39
1.928	3	5 1 1	47.10
1.924	3	-5 0 2	47.20
1.882	4	-6 1 1	48.32
1.870	3	5 2 0	48.64
1.849	2	-1 3 1	49.23
1.845	2	-3 2 2	49.36
1.8031	1	-2 3 1	50.58
1.7958	1	4 0 2	50.80
1.7769	1	2 2 2	51.38
1.7276	1L	-6 0 2	52.96
1.7141	1L	7 0 0	53.41
1.6602+	2	-1 1 3	55.29
1.6602+		3 2 2	55.29
1.6503M	2	-7 1 1	55.65
1.6503M		-2 1 3	55.65

Mercury Hydroxide Nitrate, $Hg(OH)NO_3$

Synonym
1. Mercury oxide nitrate hydrate, $Hg_2O(NO_3)_2 \cdot H_2O$

Sample
The sample was prepared by dissolving $HgNO_3 \cdot H_2O$ in a mixture of HNO_3 and H_2O. The solution was evaporated at room temperature. The first crystals formed were a mixture of phases and were discarded. The second crystals formed were used to obtain the measurements.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was determined by Ribár et al. [1971].

Lattice constants of this sample
a = 7.7438(11) Å
b = 7.1944(11)
c = 6.5893(11)
β = 114.28(1)°

a/b = 1.0764
c/b = 0.9159

Volume
334.62 $Å^3$

Density
(calculated) 5.550 g/cm^3

Figure of merit
F_{30} = 39.1 (0.013,58)

Reference intensity
$I/I_{corundum}$ = 9.2(5)

Additional pattern
1. PDF card 11-189 [Bernstein et al., 1957]

References

Bernstein, R. B., Pars, H. G., and Blumenthal, D. C. (1957). J. Am. Chem. Soc. 79, 1579.
Ribár, B., Matković, B., Sljukić, M., and Gabela, F. (1971). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 134, 311.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Ag, a = 4.08651 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
5.93	100	-1 0 1	14.93
4.614	1	0 1 1	19.22
4.583	2	-1 1 1	19.35
3.862	33	1 0 1	23.01
3.526	18	2 0 0	25.24
3.404	2	1 1 1	26.16
3.361	2	-2 1 1	26.50
3.207	32	1 2 0	27.80
3.088	18	0 2 1	28.89
3.005	19	0 0 2	29.71
2.969	19	-2 0 2	30.07
2.630	3	1 2 1	34.06
2.612	12	-2 2 1	34.31
2.582	9	-3 0 1	34.72
2.454	3	2 1 1	36.59
2.430M	11	-1 2 2	36.97
2.430M		-3 1 1	36.97
2.267	1	-3 1 2	39.73
2.236	1L	3 1 0	40.30
2.176	6	-1 0 3	41.47
2.113	5	2 2 1	42.77
2.012	4	1 2 2	45.01
1.991	5	-3 2 2	45.53
1.984	4	2 3 0	45.70
1.979	4	-3 0 3	45.82
1.970	4	3 2 0	46.04
1.937	1	3 0 1	46.86
1.930M	2	2 0 2	47.05
1.930M		0 1 3	47.05
1.9013	2	-4 0 2	47.80
1.8704	1	3 1 1	48.64
1.8547M	4	-4 1 1	49.08
1.8547M		-2 2 3	49.08
1.8378	1L	-4 1 2	49.56
1.7982	3	0 4 0	50.73
1.7641	1	4 0 0	51.78
1.7487	3	0 2 3	52.27
1.7435	2	1 4 0	52.44
1.7206	3	-1 4 1	53.19
1.7135	1	4 1 0	53.43
1.6938M	2	-4 2 1	54.10
1.6938M		-3 3 2	54.10
1.6470	1	-2 0 4	55.77
1.6298	2	1 4 1	56.41
1.6266	1	-2 4 1	56.53

Mercury Hydroxide Nitrate, $Hg(OH)NO_3$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ			2θ(°)
1.6025	1	2	4	0	57.46
1.5519	1	-4	2	3	59.52
1.5425	2	0	4	2	59.92
1.5383	2	-2	4	2	60.10
1.5204	1L	-5	0	1	60.88
1.5013	1	0	0	4	61.74
1.4978M	1L	4	1	1	61.90
1.4978M		-2	2	4	61.90
1.4874	1	-5	1	1	62.38
1.4836	1	-4	0	4	62.56
1.4743	1	-5	0	3	63.00
1.4699M	2	0	1	4	63.21
1.4699M		-1	2	4	63.21
1.4608	1	-3	2	4	63.65

CAS registry no.
12045-19-1

Sample
The sample obtained from the metallurgy Section at NBS was a mixture of ζNbB + Nb.

Color
Metallic gray

Structure
Orthorhombic, Cmcm(63), Z = 4. The structure was studied by Andersson and Kiessling [1950] and by Brewer et al., [1951]. It is isostructural with CrB.

Lattice constants of this sample

a = 3.2973(4) Å
b = 8.7229(10)
c = 3.1663(3)

a/b = 0.3780
c/b = 0.3630

Volume
91.069 $Å^3$

Density
(calculated) 7.565 g/cm^3

Figure of merit
F_{27} = 74.4(0.0095,38)

Additional pattern
1. PDF card 29-947 [Spear, K. and Blanks, Pennsylvania State University, University Park, PA].

References
Andersson, L. H. and Kiessling, R. (1950). Acta Chem. Scand. 4, 160.
Brewer, L., Sawyer, D. L., Templeton, D. H., and Dauben, C. H. (1951). J. Amer. Ceram. Soc. 34, No. 6, 173.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
4.363	7	0 2 0	20.34
3.084	46	1 1 0	28.93
2.564	80	0 2 1	34.97
2.209	100	1 1 1	40.81
2.181M	97	1 3 0	41.37
2.181M		0 4 0	41.37
1.7965M	30	1 3 1	50.78
1.7965M		0 4 1	50.78
1.6481	18	2 0 0	55.73
1.5831	13	0 0 2	58.23
1.5418M	2	2 2 0	59.95
1.5418M		1 5 0	59.95
1.4885	1	0 2 2	62.33
1.4540	6	0 6 0	63.98
1.4087	10	1 1 2	66.30
1.3863M	52	2 2 1	67.51
1.3863M		1 5 1	67.51
1.3212	8	0 6 1	71.33
1.3148	10	2 4 0	71.73
1.2808M	27	1 3 2	73.94
1.2808M		0 4 2	73.94
1.2145	6	2 4 1	78.73
1.1656	14	1 7 0	82.73
1.1419	9	2 0 2	84.84
1.1047M	2	2 2 2	88.42
1.1047M		1 5 2	88.42
1.0904+	5	2 6 0	89.89
1.0904+		0 8 0	89.89
1.0707	3	0 6 2	92.01
1.0308+	17	2 6 1	96.71
1.0308+		0 8 1	96.71
1.0283	13	3 3 0	97.03
1.0257	7	0 2 3	97.35
1.0116	8	2 4 2	99.18
.9986	6	1 1 3	100.96

Pentaerythritol, $C_5H_{12}O_4$

Synonym
1. 2,2-Bis(hydroxymethyl)-1,3-propanediol

CAS registry no.
115-77-5

Sample
The sample was obtained from Eastman Organic Chemicals, Rochester, NY. It was recrystallized from ethanol.

Color
Colorless

Structure
Tetragonal, $I\bar{4}$ (82), Z = 2. The structure was determined by Llewellyn et al. [1937] and Nitta and Watanabé [1937] and [1938a]. It was later refined by Shiono et al. [1957], [1958].

Lattice constants of this sample

a = 6.0890(12) Å
c = 8.7481(16)

c/a = 1.4367

Volume
324.34 $Å^3$

Density
(calculated) 1.394 g/cm^3

Figure of merit
F_{23} = 58.9(0.012,33)

Reference intensity
$I/I_{corundum}$ = 5.33(7)

Polymorphism
There is a cubic high temperature form stable from 179.5 °C to the melting point (260.5 °C). [Nitta and Watanabé, 1938b].

Additional pattern
1. PDF card 3-214 [Dow Chemical Co. Midland, MI]

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±	hkℓ	2θ(°)
4.998	6	1 0 1	17.73
4.371	100	0 0 2	20.30
4.306	4	1 1 0	20.61
3.068	7	1 1 2	29.08
3.044	4	2 0 0	29.32
2.632	2	1 0 3	34.04
2.601	4	2 1 1	34.46
2.499	3	2 0 2	35.90
2.186	1	0 0 4	41.26
2.153	1	2 2 0	41.93
1.991	2	2 1 3	45.53
1.9506	1	1 1 4	46.52
1.9314	2	2 2 2	47.01
1.7769	1L	2 0 4	51.38
1.7619	1L	3 1 2	51.85
1.6815	1L	1 0 5	54.53
1.6649	1	3 0 3	55.12
1.6591	1	3 2 1	55.33
1.5336	1L	2 2 4	60.30
1.4722	1L	2 1 5	63.10
1.4581	1L	0 0 6	63.78
1.4451	1L	3 1 4	64.42
1.3250	1L	3 0 5	71.09

References

Lewellyn, F. J., Cox, E. G., and Goodwin, T. H. (1937). J. Chem. Soc. London, 1937, 883.
Nitta, I. and Watanabé, T. (1937). Nature London 140, 365.
Nitta, I. and Watanabé, T. (1938a). Sci. Pap. Inst. Phys. Chem. Res. Tokyo 34, 1669.
Nitta, I. and Watanabé, T. (1938b). Bull. Chem. Soc. Japan 13, 28.
Shiono, R., Cruickshank, D. W. J., and Cox, E. G. (1957). Acta Crystallogr. 10, 794.
Shiono, R., Cruickshank, D. W. J., and Cox, E. G. (1958). Acta Crystallogr. 11, 387.

Synonym
1. Hydrazinobenzene hydrochloride

CAS registry no.
59-88-1

Sample
The sample was obtained from Eastman Kodak Co., Rochester, NY. One of the lines at 2θ = 38·96° came only within 0.06° of the calculated value.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The structure was studied by Koo [1965].

Lattice constants of this sample

a = 6.066(2) Å
b = 30.641(6)
c = 3.884(2)
β = 100.86(5)°

a/b = 0.1980
c/b = 0.1268

Volume
709.0 $Å^3$

Density
(calculated) 1.355 g/cm^3

Figure of merit
F_{30} = 13.0(0.014,172)

Reference intensity
$I/I_{corundum}$ = 1.28(14)

Reference
Koo, O. H. (1965). Bull. Chem. Soc. Jpn. 38, 262.

CuKα₁ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
15.30	100	0 2 0	5.77
7.66	22	0 4 0	11.54
5.556	30	1 2 0	15.94
4.706	22	1 4 0	18.84
3.831	90	0 8 0	23.20
3.700	20	0 2 1	24.03
3.524M	8	-1 0 1	25.25
3.524M		1 7 0	25.25
3.507	12	-1 1 1	25.38
3.417	22	0 4 1	26.06
3.224	13	1 8 0	27.65
3.065	33	0 10 0	29.11
2.977	41	2 0 0	29.99
2.924	12	2 2 0	30.55
2.901	4	-1 6 1	30.80
2.703	4	0 8 1	33.11
2.555	33	0 12 0	35.09
2.352	8	2 8 0	38.24
2.310	4	-1 10 1	38.96
2.188	1	0 14 0	41.22
2.185	2	-1 11 1	41.28
2.137M	9	2 2 1	42.26
2.137M		2 10 0	42.26
2.065	3	-2 9 1	43.81
2.034	1	2 11 0	44.51
1.938	8	2 12 0	46.83
1.9160M	3	-3 0 1	47.41
1.9160M		0 16 0	47.41
1.8234M	5	1 16 0	49.98
1.8234M		2 9 1	49.98
1.7616+	2	-1 7 2	51.86
1.7616+		1 14 1	51.86
1.7111	5	0 16 1	53.51
1.6696	1	-3 9 1	54.95
1.6370+	2	3 1 1	56.14
1.6370+		1 18 0	56.14
1.6105	1	2 16 0	57.15
1.6061M	1	-2 15 1	57.32
1.6061M		-1 17 1	57.32
1.5545	1	0 18 1	59.41
1.5323M	2	-3 12 1	60.36
1.5323M		0 20 0	60.36
1.4823M	2	4 2 0	62.62
1.4823M		-3 5 2	62.62
1.4778+	2	-4 2 1	62.83
1.4778+		2 18 0	62.83

Potassium Arsenic Fluoride, $KAsF_6$

Synonym
1. Potassium hexafluoroarsenate

CAS registry no.
17029-22-0

Sample
The sample was obtained from Alfa Inorganics, Beverly, MA.

Color
Colorless

Structure
Hexagonal, $R\bar{3}m$ (166), Z = 3. The structure was determined by Roof [1955] and refined by Ibers [1956]. It is isostructural with NH_4SbF_6.

Lattice constants of this sample

a = 7.3780(4) Å
c = 7.3095(5)

c/a = 0.9907

Volume
344.58 $Å^3$

Density
(calculated) 3.296 g/cm^3

Figure of merit
F_{30} = 100.6(0.009,32)

Reference intensity
$I/I_{corundum}$ = 3.00(8)

References

Roof, R. B. Jr., (1955). Acta Crystallogr. 8, 739.
Ibers, J. A. (1956). Acta Crystallogr. 9, 967.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} $\sigma = \pm2$	hkℓ	2θ(°)
4.810	69	1 0 1	18.43
3.684	100	1 1 0	24.14
3.170	62	0 1 2	28.13
2.927	14	0 2 1	30.52
2.436	3	0 0 3	36.87
2.405	7	2 0 2	37.36
2.293	4	2 1 1	39.26
2.1287	5	3 0 0	42.43
2.0317	7	1 1 3	44.56
2.0146	50	1 2 2	44.96
1.8445	7	2 2 0	49.37
1.7569	2	1 0 4	52.01
1.7227	5	1 3 1	53.12
1.6035	5	3 0 3	57.42
1.5947	5	3 1 2	57.77
1.5859	6	0 2 4	58.12
1.4707	3	2 2 3	63.17
1.4632	9	0 4 2	63.53
1.4571	12	2 1 4	63.83
1.4370	2	3 2 1	64.83
1.3943	6	4 1 0	67.07
1.3605	4	2 3 2	68.97
1.3293	1	2 0 5	70.83
1.2720	2	1 3 4	74.54
1.2588	1L	0 5 1	75.46
1.2506	1L	1 2 5	76.04
1.2299	3	3 3 0	77.56
1.2181	1	0 0 6	78.45
1.2101	1	4 1 3	79.07
1.2063	3	5 0 2	79.37
1.2028	3	4 0 4	79.65
1.1914	1	2 4 1	80.56
1.1570	2	1 1 6	83.48
1.1466	2	4 2 2	84.41
1.1436	2	3 2 4	84.69
1.1338	1	5 1 1	85.59
1.1279	1	3 1 5	86.15
1.0951	1L	1 5 2	89.40
1.0649	1L	6 0 0	92.66
1.0574	1	3 0 6	93.52
1.0473	1L	0 5 4	94.70
1.0398	1	4 3 1	95.60
1.0352	1L	2 3 5	96.16
1.0307	1L	1 0 7	96.73
1.0231	1L	5 2 0	97.69
1.0165	1L	2 2 6	98.54
1.0093	1L	3 4 2	99.49
1.0074	1L	2 4 4	99.75

CAS registry no.
13455-24-8

Sample
A sample labelled $KH(IO_3)_2$ was obtained from Fisher Scientific Co., Fair Lawn, N. J. It was recrystallized in water solution with the pH adjusted with I_2O_5. This γ-phase decomposes in moist air and minor amounts of another phase may be present. The reflection, d = 4.590 and I = 15 has $|2\theta_{obs} - 2\theta_{calc}| = 0.056°$.

Color
Colorless

Structure
Monoclinic, $P2_1/c$ (14), Z = 8 [Argay et al., 1969].

Lattice constants of this sample

a = 21.853(5) Å
b = 8.206(3)
c = 7.031(2)
β = 98.02(3)°

a/b = 2.6631
c/b = 0.8568

Volume
1249. $Å^3$

Density
(calculated) 4.149 g/cm^3

Figure of merit
F_{30} = 16.8(0.018,97)

Polymorphism
The monoclinic polymorph, α-$KH(IO_3)_2$, also has the space group $P2_1/a$ but a cell volume of 629.6 $Å^3$ [Argay et al., 1969].

Additional pattern
1. Argay et al. [1969]

References
Argay, Gy., Náray-Szabó, I., and Péter, É. (1969). J. Therm. Anal. 1, 413.

CuKα$_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
10.87	1L	2 0 0	8.13
6.55	1L	2 1 0	13.50
5.41M	41	3 1 0	16.38
5.41M		4 0 0	16.38
5.32	21	0 1 1	16.66
5.03	5	1 1 1	17.61
4.591	15	2 1 1	19.32
4.526	10	4 1 0	19.60
4.075	5	3 1 1	21.79
4.032	7	1 2 0	22.03
4.005	2	-4 1 1	22.18
3.831M	9	2 2 0	23.20
3.831M		5 1 0	23.20
3.602M	60	6 0 0	24.70
3.602M		4 1 1	24.70
3.530M	20	0 2 1	25.21
3.530M		-1 2 1	25.21
3.481	42	0 0 2	25.57
3.457	45	-2 0 2	25.75
3.268M	100	4 2 0	27.27
3.268M		-3 2 1	27.27
3.186M	44	2 0 2	27.98
3.186M		-2 1 2	27.98
3.142	18	-6 1 1	28.38
3.135	17	-4 0 2	28.45
3.089M	41	7 0 0	28.88
3.089M		3 2 1	28.88
2.978M	5	5 2 0	29.98
2.978M		3 0 2	29.98
2.807	5	-7 1 1	31.85
2.759	1	4 0 2	32.43
2.705	18	8 0 0	33.09
2.649M	19	2 3 0	33.81
2.649M		5 2 1	33.81
2.567M	4	8 1 0	34.92
2.567M		-6 1 2	34.92
2.556M	4	3 3 0	35.08
2.556M		7 1 1	35.08
2.522	2	-8 1 1	35.57
2.432	3	5 1 2	36.93
2.411M	1L	-7 2 1	37.26
2.411M		3 2 2	37.26
2.347	5	6 0 2	38.32
2.313M	3	8 1 1	38.90
2.313M		5 3 0	38.90

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
2.283	1L	-9 1 1	39.43
2.250	4	7 2 1	40.04
2.163M	2	10 0 0	41.72
2.163M		5 2 2	41.72
2.133M	3	-6 3 1	42.35
2.133M		2 1 3	42.35
2.107	2	9 1 1	42.89
2.092	3	10 1 0	43.22
2.075M	6	2 3 2	43.59
2.075M		9 2 0	43.59
2.057M	28	-9 2 1	43.99
2.057M		3 1 3	43.99
2.054	25	-9 1 2	44.05
2.034	24	-1 2 3	44.51
2.004M	9	8 0 2	45.22
2.004M		-8 2 2	45.22
1.989	4	1 2 3	45.58
1.924+	7	8 3 0	47.20
1.924+		2 4 1	47.20
1.912+	5	-11 1 1	47.52
1.912+		-10 1 2	47.52
1.803	3	12 0 0	50.59
1.783+	9	11 1 1	51.19
1.783+		6 4 0	51.19
1.768	7	0 4 2	51.67
1.763	6	-3 3 3	51.83
1.750	9	5 2 3	52.23
1.729	8	-4 0 4	52.91
1.725	7	2 4 2	53.06
1.717+	4	2 3 3	53.30
1.717+		-4 4 2	53.30
1.701	4	-12 0 2	53.85
1.682	5	2 0 4	54.52
1.679M	4	1 1 4	54.60
1.679M		-5 4 2	54.60
1.669M	5	-10 1 3	54.96
1.669M		11 2 1	54.96
1.6484M	4	-9 2 3	55.72
1.6484M		2 1 4	55.72
1.6338M	7	8 4 0	56.26
1.6338M		-6 4 2	56.26
1.5962+	2	10 2 2	57.71
1.5962+		-10 3 2	57.71
1.5448+	1L	-4 5 1	59.82
1.5448+		6 4 2	59.82

Potassium Hydrogen Oxalate Hydrate, $C_4H_3KO_8 \cdot 2H_2O$

Synonyms
1. Potassium trihydrogen oxalate dihydrate
2. Potassium tetroxalate

CAS registry no.
6100-20-5

Sample
NBS Standard Reference Material #189.

Color
Colorless

Structure
Triclinic, $P\bar{1}$ (2), Z = 2. The structure was determined by Haas (1964).

Lattice constants of this sample

a = 7.031(2) Å
b = 10.611(4)
c = 6.367(2)
α = 101.36(3)°
β = 100.18(2)
γ = 93.82(2)

a/b = 0.6626
c/b = 0.6000

Volume
455.8 Å^3

Density
(calculated) 1.852 g/cm^3

Figure of merit
F_{30} = 40.6(0.017,44)

Reference intensity
$I/I_{corundum}$ = 1.14(7)

Additional pattern
1. PDF card 14-845 [Dow Chemical Co., Midland, Michigan]

Reference
Haas, D. J. (1964). Acta Crystallogr. 17, 1511.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
6.13	9	0 0 1	14.43
6.04	8	-1 1 0	14.66
5.85	1	0 -1 1	15.14
5.47	1	1 1 0	16.18
5.101	2	-1 0 1	17.37
4.841	14	0 1 1	18.31
4.767	5	-1 -1 1	18.60
4.451	13	0 -2 1	19.93
4.367	3	-1 2 0	20.32
4.197	3	1 -1 1	21.15
3.943	3	1 2 0	22.53
3.828	2	-1 -2 1	23.22
3.626	1	1 1 1	24.53
3.597	2	0 2 1	24.73
3.458	5	-1 2 1	25.74
3.446	5	0 3 0	25.83
3.440	4	2 0 0	25.88
3.376	3	-2 1 0	26.38
3.321	3	0 -3 1	26.82
3.283	4	-2 0 1	27.14
3.143	100	-2 -1 1	28.37
3.123	76	0 -1 2	28.56
3.064	28	0 0 2	29.12
3.041	7	-1 -1 2	29.35
2.990	7	1 -3 1	29.86
2.963M	7	1 2 1	30.14
2.963M		1 3 0	30.14
2.921	1	0 -2 2	30.58
2.820	8	-1 -2 2	31.71
2.790	27	-2 -2 1	32.05
2.783	22	-1 1 2	32.14
2.757	9	-2 2 1	32.45
2.658	7	2 -2 1	33.69
2.578M	12	0 -3 2	34.77
2.578M		1 -2 2	34.77
2.544	4	-2 0 2	35.25
2.531	7	-2 -1 2	35.44
2.509	5	-1 4 0	35.76
2.483	3	-1 -3 2	36.15
2.442M	20	-1 2 2	36.78
2.442M		1 -4 1	36.78
2.426	6	1 3 1	37.03
2.412	6	1 1 2	37.25
2.394	4	-2 -3 1	37.54
2.384	5	2 -3 1	37.70
2.361	13	-2 3 1	38.08
2.348	8	1 -3 2	38.30
2.342	6	1 4 0	38.40
2.316	3	2 3 0	38.85
2.281	7	2 2 1	39.48
2.257	2	-3 1 1	39.91
2.232	6	-3 -1 1	40.37
2.199	3	-2 2 2	41.01
2.184	5	-3 2 0	41.30
2.146	7	-1 -4 2	42.07

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
2.100M	2	2 -2 2	43.04
2.100M		0 -5 1	43.04
2.094	3	2 0 2	43.17
2.083	2	-3 -2 1	43.41
2.068M	4	-1 0 3	43.73
2.068M		0 5 0	43.73
2.053	5	0 -2 3	44.07
2.049	3	3 -1 1	44.16
2.040M	3	0 0 3	44.36
2.040M		-1 5 0	44.36
2.015	2	-3 -1 2	44.94
2.009	2	-3 3 0	45.09
1.998	7	3 -2 1	45.35

Synonym
1. Potassium niobate

CAS registry no.
12030-85-2

Sample
The sample was a Johnson Matthey chemical obtained from Ventron Corp., Danvers, MA.

Major impurities
The manufacturer's spectrographic analysis showed ≈ 3 ppm silicon.

Color
Colorless

Structure
Orthorhombic, Cm2m (38), Z = 2, isostructural with the distorted perovskite form of $BaTiO_3$. The structure was determined by Katz and Megaw [1954].

Lattice constants of this sample

a = 5.6950(4) Å
b = 5.7213(3)
c = 3.9739(2)

a/b = 0.9954
c/b = 0.6946

Volume
129.48 $Å^3$

Density
(calculated) 4.167 g/cm^3

Figure of merit
F_{30} = 96.0(0.009,35)

Reference intensity
$I/I_{corundum}$ = 5.26(12)

Polymorphism
Potassium niobium oxide crystallizes in three modifications, orthorhombic at room temperature, changing to tetragonal at about 255 °C and cubic near 435 °C [Wood, 1951].

Additional pattern
1. PDF card 9-156 [Wood, priv. comm.]

References
Katz, L. and Megaw, H. D. (1967). Acta Crystallogr. 22, 639.
Wood, E. A. (1951). Acta Crystallogr. 4, 353.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
4.035	47	1 1 0	22.01
3.973	22	0 0 1	22.36
2.859	36	0 2 0	31.26
2.848	46	2 0 0	31.39
2.832	100	1 1 1	31.57
2.322	1	0 2 1	38.75
2.0180	33	2 2 0	44.88
1.9866	16	0 0 2	45.63
1.8081	3	1 3 0	50.43
1.7998	9	2 2 1	50.68
1.7831	6	1 1 2	51.19
1.6462	15	1 3 1	55.80
1.6413	19	3 1 1	55.98
1.6314	11	0 2 2	56.35
1.6296	6	2 0 2	56.42
1.4305	2	0 4 0	65.16
1.4239	4	4 0 0	65.50
1.4160	13	2 2 2	65.91
1.3458M	1	0 4 1	69.83
1.3458M		3 3 0	69.83
1.3405	1	4 0 1	70.15
1.3371	2	1 3 2	70.35
1.3347	2	3 1 2	70.50
1.3249	1L	0 0 3	71.10
1.2782	2	2 4 0	74.12
1.2746M	7	4 2 0	74.36
1.2746M		3 3 1	74.36
1.2586	4	1 1 3	75.47
1.2169	1L	2 4 1	78.54
1.2137	1L	4 2 1	78.79
1.2020	1L	0 2 3	79.71
1.1610	2	0 4 2	83.13
1.1576	3	4 0 2	83.43
1.1221	1L	1 5 0	86.70
1.1170	1L	5 1 0	87.20
1.1142	1L	3 3 2	87.47
1.1075	1L	2 2 3	88.14
1.0797	1	1 5 1	91.03
1.0751M	3	5 1 1	91.53
1.0751M		2 4 2	91.53
1.0727	3	4 2 2	91.79
1.0687	3	1 3 3	92.24
1.0674	2	3 1 3	92.38
1.0091	1	4 4 0	99.52
.9934	1L	0 0 4	101.68

Potassium Niobium Oxide, $KNbO_3$ - (continued)

d(Å)	I^{rel} $\sigma = \pm 1$	hkℓ	2θ(°)
.9801	1L	3 5 0	103.62
.9780M	1L	4 4 1	103.93
.9780M		5 3 0	103.93
.9769	1L	1 5 2	104.10
.9738	1L	5 1 2	104.57
.9696	1L	4 0 3	105.20
.9646	1L	1 1 4	105.99
.9534	1L	0 6 0	107.79
.9514	1	3 5 1	108.13
.9494M	2	5 3 1	108.46
.9494M		6 0 0	108.46
.9438	1	3 3 3	109.41
.9381	1	2 0 4	110.40
.9272	1L	0 6 1	112.35
.9231	1L	6 0 1	113.12
.9197	1L	2 4 3	113.76

Synonym
1. Potassium persulfate

CAS registry no.
7727-21-1

Sample
The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ. and was recrystallized from an aqueous solution.

Color
Colorless

Structure
Triclinic, Z = 1 (assuming a density near 2.5). The cell was obtained by V. Himes using a single crystal on a diffractometer. The cell was confirmed by the Visser program [1969]. Two somewhat different triclinic cells were reported in the literature [Keen, 1935 and Gerstäcker et al., 1928]. Our data did not index on either of these cells.

Lattice constants of this sample

a = 5.514(2) Å
b = 7.038(2)
c = 5.116(2)
α = 106.11(2)°
β = 90.15(3)
γ = 106.30(3)

a/b = 0.7835
c/b = 0.7269

Volume
182.38 $Å^3$

Density
(calculated) 2.461 g/cm^3
(measured) 2.45 g/cm^3

Figures of merit
F_{30} = 34.9(0.016,52)
M_{20} = 27.3

Reference intensity
$I/I_{corundum}$ = 1.31(7)

Additional pattern
1. PDF card 12-483 [Institute of Physics, University College, Cardiff, Wales].

References
Gerstäcker, A., Möller, H., and Reis, A. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 66, 421.
Keen, R. C. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 91, 129.
Visser, J. W. (1969). J. Appl. Crystallogr.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
5.27	2	1 0 0	16.80
4.892	15	0 0 1	18.12
4.847	20	-1 1 0	18.29
4.602	1L	0 -1 1	19.27
3.750	9	-1 0 1	23.71
3.699	38	1 -1 1	24.04
3.603	4	1 1 0	24.69
3.443	52	1 0 1	25.86
3.268	56	-1 -1 1	27.27
3.232M	100	0 2 0	27.58
3.232M		-1 1 1	27.58
3.153	3	0 -2 1	28.28
3.025	11	1 -2 1	29.50
2.736	14	-2 1 0	32.71
2.634M	9	1 1 1	34.01
2.634M		2 0 0	34.01
2.548	10	0 -1 2	35.20
2.466	22	-1 -2 1	36.40
2.419	10	-2 2 0	37.13
2.397	5	0 2 1	37.49
2.358	3	-2 1 1	38.14
2.315	3	1 -1 2	38.87
2.297+	5	-1 0 2	39.18
2.297+		2 -2 1	39.18
2.273M	3	1 -3 1	39.62
2.273M		-1 -1 2	39.62
2.239M	2	2 0 1	40.25
2.239M		-1 3 0	40.25
2.224M	1	0 -3 1	40.52
2.224M		2 1 0	40.52
2.154	3	0 3 0	41.90
2.098	1	0 1 2	43.08
1.995	5	1 2 1	45.42
1.975M	7	-2 3 0	45.91
1.975M		2 -3 1	45.91
1.923	10	1 -3 2	47.22
1.917	4	0 -3 2	47.39
1.881	7	-1 -3 1	48.35
1.858	2	-1 3 1	48.98
1.853	2	2 -2 2	49.14
1.844	1	1 1 2	49.39
1.809	5	-2 -1 2	50.40
1.800	7	2 2 0	50.66
1.753	2	1 -4 1	52.14
1.711	3	3 -2 1	53.51

d(Å)	I^{rel} σ = ±4	hkℓ	2θ(°)
1.6338M	3	-3 2 1	56.26
1.6338M		-2 -2 2	56.26
1.6154M	8	1 -2 3	56.96
1.6154M		1 -1 3	56.96
1.6138M	4	1 -4 2	57.02
1.6138M		-2 2 2	57.02

CAS registry no.
12007-34-0

Sample
The sample was obtained from Cerac, Menomonee Falls, WI.

Color
Metallic gray

Structure
Hexagonal, P6/mmm (191) Z = 1. The structure was qualitatively done by Zhuravlev and Stepanova [1958].

Lattice constants of this sample

a = 3.14573(12) Å
c = 3.5175(2)

c/a = 1.1182

Volume
30.145 $Å^3$

Density
(calculated) 3.667 g/cm^3

Figure of merit
F_{19} = 73.3(0.011,23)

Additional pattern
1. PDF card 11-527 [Zhuravlev and Stepanova, 1958].

References
Zhuravlev, N. N. and Stepanova, A. A. (1958). Kristallografiya 3, 83.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
3.517	17	0 0 1	25.30
2.725	51	1 0 0	32.84
2.153	100	1 0 1	41.92
1.7594	10	0 0 2	51.93
1.5733	18	1 1 0	58.63
1.4774	13	1 0 2	62.85
1.4358	8	1 1 1	64.89
1.3619	5	2 0 0	68.89
1.2703	12	2 0 1	74.66
1.1721M	12	0 0 3	82.17
1.1721M		1 1 2	82.17
1.0768M	8	1 0 3	91.34
1.0768M		2 0 2	91.34
1.0297	3	2 1 0	96.85
.9883	8	2 1 1	102.42
.9401	1L	1 1 3	110.05
.9081	3	3 0 0	116.05
.8885M	6	2 0 3	120.21
.8885M		2 1 2	120.21
.8792M	2	0 0 4	122.35
.8792M		3 0 1	122.35
.8369	2	1 0 4	133.99
.8069	3	3 0 2	145.36

Silver Mercury Iodide, β-Ag_2HgI_4

CAS registry no.
7784-03-4

Sample
The sample was obtained from Ventron Corp. (Alfa), Danvers, MA.

Color
Vivid yellow

Structure
Tetragonal, $I\bar{4}$ (82), Z = 2, pseudocubic. The structure of β-Ag_2HgI_4 was determined by Hahn et al. [1955]. A cell with c/2 was reported by Ketelaar [1931] and a cell with 2a was reported by Frevel and North [1950].

Lattice constants of this sample
a = 6.3302(8) Å
c = 12.624(2)

c/a = 1.9942

Volume
505.88 $Å^3$

Density
(calculated) 6.069 g/cm^3

Figure of merit
F_{30} = 47.1(0.016,41)

Reference intensity
$I/I_{corundum}$ = 5.60(10)

Polymorphism
Above 60 °C, Ag_2HgI_4 is cubic [Ketelaar, 1931]. Otsubo [1966] reports another form of Ag_2HgI_4 as hexagonal and stable above 165 °C.

Additional patterns
1. PDF card 3-0949 [Ketelaar, 1931]
2. PDF card 4-0442 [Frevel and North, 1950]
3. PDF card 18-1183 [Hahn et al., 1955]

References

Frevel, L. K. and North, P. P. (1950). J. Appl. Phys. 21, 1038.
Hahn, H., Frank, G., and Klingler, W. (1955). Z. Anorg. Allgem. Chem. 279, 271.
Ketelaar, J. A. A. (1931). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 80, 192.
Otsubo, Y., Nitta, A., Kaneko, M., Iwata, Y., and Ueki, A. (1966). Kogyo Kagaku Zasshi 69, 1716.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
6.30	3	0 0 2	14.05
5.64	6	1 0 1	15.69
4.471	6	1 1 0	19.84
3.650	100	1 1 2	24.37
3.502	5	1 0 3	25.41
3.163	1L	2 0 0	28.19
3.156	1L	0 0 4	28.25
2.828	5	2 0 2	31.61
2.761	5	2 1 1	32.40
2.578	4	1 1 4	34.77
2.347M	3	2 1 3	38.32
2.347M		1 0 5	38.32
2.236	45	2 0 4	40.31
2.103	2	0 0 6	42.97
2.081	2	3 0 1	43.46
2.002	1	3 1 0	45.27
1.908	19	3 1 2	47.62
1.904	18	1 1 6	47.72
1.884	1	2 1 5	48.26
1.7385	1L	3 2 1	52.60
1.7340	1L	1 0 7	52.75
1.6907	1L	3 1 4	54.21
1.6203	1	3 2 3	56.77
1.5829	3	4 0 0	58.24
1.5782	3	0 0 8	58.43
1.5332	1	2 2 6	60.32
1.5240	1L	4 1 1	60.72
1.5206	1L	2 1 7	60.87
1.4887	1L	1 1 8	62.32
1.4508	4	3 1 6	64.14
1.4416M	2	4 1 3	64.60
1.4416M		3 2 5	64.60
1.3813	1L	4 2 2	67.79
1.3494	1L	3 3 4	69.62
1.3119	1L	4 1 5	71.91
1.2917	4	4 2 4	73.22
1.2901	3	2 2 8	73.32
1.2643	1L	4 0 6	75.07

Synonym
1. Sodium perchlorate hydrate

CAS registry no.
7791-07-3

Sample
The sample was recrystallized from reagent material received from the Fisher Scientific Co., Fair Lawn, NJ. The crystals were very unstable, changing readily to the anhydrous phase and back again depending on the atmospheric relative humidity.

*Because of the sample's instability, the intensities were calculated from the structure data given by Berglund et al. [1975].

Color
Colorless

Structure
Monoclinic, C2/c (15), Z = 8. The structure was refined by Berglund et al. [1975].

Lattice constants of this sample

a = 15.555(3) Å
b = 5.5436(9)
c = 11.063(3)
β = 110.70(2)°

a/b = 2.8059
c/b = 1.9956

Volume
892.4 $Å^3$

Density
(calculated) 2.091 g/cm^3

Figure of merit
F_{30} = 26.0 (0.015,78)

Reference intensity
$I/I_{corundum}$ = 1.34 (calculated from the structural data)

Additional pattern
1. PDF card 28-1071 [Hanawalt et al., [1938]

References
Berglund, B., Thomas, J. O., and Tellgren, R. (1975). Acta Crystallogr. B31, 1842.
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I*	hkℓ	2θ(°)
5.18M	44	1 1 0	17.10
5.18M		0 0 2	17.10
4.894	2	-1 1 1	18.11
4.421	6	1 1 1	20.07
3.648+	77	2 0 2	24.38
3.648+		3 1 0	24.38
3.445M	100	1 1 2	25.84
3.445M		-3 1 2	25.84
3.187	5	3 1 1	27.97
2.928	3	-3 1 3	30.51
2.771	9	0 2 0	32.28
2.764	11	-2 0 4	32.36
2.707	3	-5 1 1	33.06
2.666	4	3 1 2	33.59
2.660	3	-5 1 2	33.66
2.592M	1	-2 2 1	34.58
2.592M		2 2 0	34.58
2.585M	1L	0 0 4	34.67
2.585M		-4 0 4	34.67
2.577M	1L	4 0 2	34.78
2.577M		5 1 0	34.78
2.467	1	-5 1 3	36.39
2.443+	5	0 2 2	36.76
2.443+		-2 2 2	36.76
2.437	5	-3 1 4	36.86
2.228	1	3 1 3	40.45
2.205+	16	4 2 0	40.90
2.205+		2 0 4	40.90
2.162	1	0 2 3	41.75
2.063	4	5 1 2	43.85
2.060	3	-7 1 2	43.92
2.040	1	-7 1 1	44.36
2.011	1	-1 1 5	45.04
1.958M	1	-2 2 4	46.33
1.958M		2 2 3	46.33
1.947M	1	6 0 2	46.61
1.947M		7 1 0	46.61
1.885M	2	-6 2 2	48.23
1.885M		-6 2 1	48.23
1.844	1L	1 1 5	49.39
1.825M	7	4 0 4	49.93
1.825M		6 2 0	49.93
1.820M	8	-8 0 4	50.07
1.820M		-1 3 1	50.07
1.811	1L	5 1 3	50.35
1.792	1L	1 3 1	50.92
1.739	2	-3 3 1	52.57
1.724M	9	0 0 6	53.08
1.724M		-6 2 4	53.08
1.722M	8	-6 0 6	53.16

d(Å)	I*	hkℓ			2θ(°)
1.722M		6	2	1	53.16
1.7040M	1	1	3	2	53.75
1.7040M		-3	3	2	53.75
1.7017M	3	-1	1	6	53.83
1.7017M		-4	2	5	53.83
1.6691	1	3	3	1	54.97
1.6497M	1L	7	1	2	55.67
1.6497M		-1	3	3	55.67
1.5919	1	-8	2	2	57.88
1.5794M	1	3	3	2	58.38
1.5794M		-5	3	2	58.38
1.5514M	1L	9	1	0	59.54
1.5514M		-10	0	2	59.54
1.5254M	1	2	2	5	60.66
1.5254M		4	2	4	60.66
1.5202	2	8	2	0	60.89
1.5126	1L	-9	1	5	61.23
1.5006M	1L	5	3	1	61.77
1.5006M		-5	1	7	61.77
1.4199M	2	3	1	6	65.71
1.4199M		-7	3	2	65.71
1.4162	3	-3	3	5	65.90
1.3860	1	0	4	0	67.53
1.3816M	2	7	3	0	67.77
1.3816M		4	0	6	67.77
1.3734	1	0	4	1	68.23
1.3631	1	-11	1	2	68.82
1.3543+	1	7	1	4	69.33
1.3543+		8	2	2	69.33
1.3385+	1L	-2	4	2	70.27
1.3385+		2	4	1	70.27
1.3342M	1	-11	1	1	70.53
1.3342M		6	2	4	70.53
1.3309M	1	-10	2	4	70.73
1.3309M		-10	2	1	70.73
1.2953M	1	-4	4	2	72.98
1.2953M		4	4	0	72.98

Synonym
1. Monosodium glutamate hydrate
2. Accent

CAS registry no.
142-47-2

Sample
The sample was manufactured by the Ajinomoto Co., Japan, and purchased as a food additive. It was recrystallized from a mixture of water and ethanol.

Color
Colorless

Structure
Orthorhombic, $P2_12_12_1(19)$, Z = 8. The unit cell and space group were determined by Uno [1952].

Lattice constants of this sample

a = 15.235(3) Å
b = 17.937(4)
c = 5.667(2)

a/b = 0.8494
c/b = 0.3104

Volume
1521.3 $Å^3$

Density
(calculated) 1.634 g/cm^3

Figure of merit
F_{30} = 45.6(0.014,48)

Reference intensity
$I/I_{corundum}$ = 0.35(2)

Additional pattern
1. PDF card 18-1904 [Institute of Physics, University College, Cardiff, Wales]

Reference
Uno, T., (1952). Yokugaku Zasshi (J. Pharm. Soc. Japan) 72, 26.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
11.62	3	1 1 0	7.60
8.95	10	0 2 0	9.87
7.72	10	1 2 0	11.46
7.61	4	2 0 0	11.62
7.02	3	2 1 0	12.60
5.80	15	2 2 0	15.27
5.562	5	1 3 0	15.92
5.024	8	1 1 1	17.64
4.886	2	3 1 0	18.14
4.697	4	2 3 0	18.88
4.519	95	1 2 1	19.63
4.416	75	3 2 0	20.09
4.358	39	2 1 1	20.36
4.298	6	1 4 0	20.65
4.017	38	2 2 1	22.11
3.935	24	1 3 1	22.58
3.860	32	2 4 0	23.02
3.807	88	4 0 0	23.35
3.728	33	4 1 0	23.85
3.589	33	2 3 1	24.79
3.505	100	4 2 0	25.39
3.460	17	3 2 1	25.73
3.402	18	1 4 1	26.17
3.361	12	3 4 0	26.50
3.209	24	4 3 0	27.78
3.175M	74	3 3 1	28.08
3.175M		2 4 1	28.08
3.141	19	4 0 1	28.39
3.096	19	4 1 1	28.81
2.958	16	1 5 1	30.19
2.931M	8	1 6 0	30.47
2.931M		3 5 0	30.47
2.901	19	4 4 0	30.80
2.879	37	3 4 1	31.04
2.802	16	2 5 1	31.91
2.784+	8	0 0 2	32.12
2.784+		2 6 0	32.12
2.715	2	5 3 0	32.97
2.706	2	1 1 2	33.08
2.642	9	5 1 1	33.90
2.633	14	0 6 1	34.02
2.612M	25	2 0 2	34.30
2.612M		4 5 0	34.30
2.593M	29	1 6 1	34.57
2.593M		3 5 1	34.57

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
2.562	7	5 2 1	35.00
2.525M	9	1 7 0	35.53
2.525M		0 3 2	35.53
2.521	9	5 4 0	35.58
2.489M	26	1 3 2	36.06
2.489M		2 6 1	36.06
2.441+	16	6 2 0	36.79
2.441+		3 0 2	36.79
2.362	11	4 5 1	38.06
2.356	12	3 2 2	38.16
2.352	17	4 6 0	38.24
2.338+	9	3 6 1	38.48
2.338+		6 3 0	38.48
2.310	8	6 0 1	38.96
2.301	16	1 7 1	39.11
2.296	17	5 4 1	39.21
2.258M	16	3 3 2	39.90
2.258M		2 4 2	39.90
2.237	24	6 2 1	40.28
2.230	22	4 1 2	40.42
2.227	19	2 7 1	40.48
2.200	12	0 5 2	41.00
2.167	41	4 6 1	41.65
2.144M	6	3 4 2	42.12
2.144M		5 5 1	42.12
2.135	4	5 6 0	42.29
2.126	4	4 7 0	42.49
2.115M	6	3 7 1	42.71
2.115M		7 2 0	42.71
2.060	5	1 8 1	43.92
2.052	9	3 8 0	44.10
2.037	4	0 6 2	44.44
1.994	7	5 6 1	45.46
1.987	5	4 7 1	45.62
1.959	7	7 4 0	46.31

Sodium Hydrogen Oxalate Hydrate, $C_2HNaO_4 \cdot H_2O$

Synonym
1. Sodium binoxalate hydrate
2. Sodium acid oxalate hydrate

CAS registry no.
16009-94-2

Sample
The sample was obtained from Fisher Scientific Co., Fair Lawn, N. J. It was recrystallized from a hot aqueous solution to which a small amount of $H_2C_2O_4$ was added. The sample was mounted in Canada Balsam for the intensity measurements. Since the material exhibited strong cleavage and a tendency to lose H_2O, the intensity determinations may be subject to some error.

Color
Colorless

Structure
Triclinic, $P\bar{1}$ (2), Z = 2 [Hendricks, 1935].

Lattice constants of this sample

a = 6.516(2) Å
b = 6.675(2)
c = 5.708(2)
α = 95.06(4)°
β = 109.96(4)
γ = 75.03(2)

a/b = 0.9762
c/b = 0.8551

Volume
225.43 $Å^3$

Density
(calculated) 1.916 g/cm^3

Figure of merit
F_{30} = 26.2(0.016,71)

Additional pattern
1. PDF card 14-755 [Hanawalt et al., 1938]

References
Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Hendricks, S. B. (1935). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 92, 301.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
6.44	4	0 1 0	13.73
5.93	1L	1 0 0	14.92
5.36	14	0 0 1	16.53
5.027	3	1 1 0	17.63
4.862	14	-1 0 1	18.23
4.318	11	-1 -1 1	20.55
4.132M	10	0 -1 1	21.49
4.132M		0 1 1	21.49
3.919	10	-1 1 0	22.67
3.226	14	0 2 0	27.63
3.179	12	1 2 0	28.05
3.084	4	-2 -1 1	28.93
2.987	32	2 1 0	29.89
2.968	100	2 0 0	30.08
2.683	21	0 0 2	33.37
2.583	6	-1 2 0	34.70
2.568	1L	-2 -2 1	34.91
2.530	7	-2 1 1	35.45
2.482	24	-1 1 2	36.16
2.477+	18	0 -1 2	36.24
2.477+		0 1 2	36.24
2.442	8	-2 -1 2	36.77
2.306	3	2 1 1	39.03
2.256	5	-1 -2 2	39.93
2.165	8	-3 -1 1	41.69
2.131M	9	1 1 2	42.39
2.131M		-1 -3 1	42.39
2.097	6	-3 0 1	43.10
2.063+	7	2 2 1	43.84
2.063+		0 -2 2	43.84
2.012+	2	-3 -2 1	45.02
2.012+		-1 2 2	45.02
1.959	7	-2 2 0	46.32
1.906	5	3 2 0	47.67
1.893	1L	-1 0 3	48.01
1.858M	3	-3 1 1	49.00
1.858M		-1 -1 3	49.00
1.835	4	-1 3 1	49.64
1.780	4	-1 1 3	51.28
1.7416M	5	-3 -3 1	52.50
1.7416M		2 3 1	52.50
1.7270	13	2 0 2	52.98
1.6852	1L	3 0 1	54.40
1.6610	9	1 4 0	55.26
1.6408	2	-3 -3 2	56.00

Sodium Iodate Hydrate, $NaIO_3 \cdot H_2O$

Synonym
1. Sodium iodate monohydrate

CAS registry no.
22451-04-3

Sample
The sample was crystallized by slow evaporation of an aqueous solution of $NaIO_3$. The material was somewhat unstable; thus, the intensity measurements may be slightly in error.

Color
Colorless

Structure
Orthorhombic, $P22_12$ (17), Z = 8, assuming a density near 2.5. Indexed by use of the Visser program. The space group was assumed, based on the consideration of the absent reflections.

Lattice constants of this sample

a = 9.065(3) Å
b = 16.632(5)
c = 7.638(2)

a/b = 0.5450
c/b = 0.4592

Volume
1151.6 Å^3

Density
(calculated) 2.491 g/cm^3

Figures of merit
F_{30} = 18.7(0.013,120)
M_{20} = 12.2

Reference intensity
$I/I_{corundum}$ = 2.42(14)

Additional pattern
1. PDF card 1-156 [Hanawalt et al., 1938]

References

Hanawalt, J. D., Rinn, H. W., and Frevel, L. K. (1938). Ind. Eng. Chem. Anal. Ed. 10, 457.
Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ	2θ(°)
6.93	76	0 1 1	12.77
5.836	100	1 0 1	15.17
4.774	25	1 2 1	18.57
3.976	62	2 2 0	22.34
3.792	8	2 1 1	23.44
3.441	84	1 1 2	25.87
3.189	39	2 3 1	27.96
3.021	85	3 0 0	29.55
2.971M	44	3 1 0	30.05
2.971M		1 3 2	30.05
2.919	8	2 0 2	30.60
2.890	19	1 5 1	30.92
2.771M	20	0 6 0	32.28
2.771M		3 1 1	32.28
2.661	25	3 2 1	33.65
2.654M	13	3 3 0	33.74
2.654M		1 6 0	33.74
2.449	4	1 0 3	36.67
2.391	12	2 4 2	37.59
2.345	9	3 1 2	38.35
2.328	3	3 4 1	38.64
2.314	5	0 3 3	38.88
2.279	23	3 2 2	39.51
2.243M	11	0 6 2	40.17
2.243M		1 3 3	40.17
2.201M	4	1 7 1	40.97
2.201M		2 1 3	40.97
2.144	4	2 2 3	42.11
2.112	14	1 4 3	42.78
2.023M	6	4 3 1	44.77
2.023M		0 5 3	44.77
2.017	7	0 7 2	44.91
2.011	7	2 6 2	45.05
1.989	5	4 4 0	45.56
1.969	26	1 7 2	46.05
1.930	7	3 5 2	47.04
1.8976M	4	4 2 2	47.90
1.8976M		0 1 4	47.90
1.8744	10	0 6 3	48.53
1.8469	4	2 5 3	49.30
1.8344	13	2 8 1	49.66
1.8196	4	4 5 1	50.09
1.7708M	11	5 2 0	51.57
1.7708M		1 3 4	51.57
1.7497	9	2 1 4	52.24
1.7355	6	0 4 4	52.70
1.7218	7	2 2 4	53.15
1.6846	8	4 1 3	54.42

Synonym
1. Sodium thiosulfate pentahydrate

CAS registry no.
10102-17-7

Sample
The sample was obtained from the Fisher Scientific Co., Fair Lawn, NJ.

Color
Colorless

Structure
Monoclinic, $P2_1/a$ (14), Z = 4. The structure of $Na_2S_2O_3 \cdot 5H_2O$ was determined by Taylor and Beevers [1952].

Lattice constants of this sample

a = 7.5361(14) Å
b = 21.595(6)
c = 5.9503(12)
β = 103.80(2)°

a/b = 0.3490
c/b = 0.2755

Volume
940.4 $Å^3$

Density
(calculated) 1.753 g/cm³

Figure of merit
F_{30} = 52.3(0.012,47)

Additional pattern
1. PDF card 13-528 [University College, Cardiff, Wales]

Reference
Taylor, P. G. and Beevers, C. A. (1952). Acta Crystallogr. 5, 341.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
10.79	4	0 2 0	8.19
6.93	5	1 1 0	12.76
6.05	19	1 2 0	14.62
5.775	32	0 0 1	15.33
5.580	24	0 1 1	15.87
5.401	100	0 4 0	16.40
5.125	15	1 3 0	17.29
5.024	20	-1 1 1	17.64
4.665	19	-1 2 1	19.01
4.507	23	0 3 1	19.68
4.339	5	1 4 0	20.45
4.205	28	-1 3 1	21.11
4.010	4	1 1 1	22.15
3.945	11	0 4 1	22.52
3.823	31	1 2 1	23.25
3.660	35	2 0 0	24.30
3.601	16	0 6 0	24.70
3.552	25	1 3 1	25.05
3.490	16	-2 0 1	25.50
3.446	27	-2 1 1	25.83
3.324	46	-2 2 1	26.80
3.258M	2	2 3 0	27.35
3.258M		1 4 1	27.35
3.141	35	-2 3 1	28.39
3.031	2	2 4 0	29.45
2.957	60	-1 6 1	30.20
2.911	35	-1 1 2	30.69
2.864	37	0 1 2	31.20
2.843	34	1 7 0	31.44
2.794M	55	2 5 0	32.01
2.794M		0 2 2	32.01
2.721M	10	0 7 1	32.89
2.721M		-1 3 2	32.89
2.648	1	-1 7 1	33.82
2.613	9	2 3 1	34.29
2.586	8	-2 0 2	34.66
2.566	6	2 6 0	34.94
2.548	6	0 4 2	35.20
2.532	7	1 8 0	35.42
2.506	13	-2 6 1	35.80
2.489	8	2 4 1	36.06
2.451	47	-3 1 1	36.64
2.428M	20	-1 5 2	36.99
2.428M		1 2 2	36.99
2.355	16	1 3 2	38.19
2.335M	3	-3 3 1	38.52
2.335M		-2 4 2	38.52
2.275	6	-1 6 2	39.58
2.263	10	1 4 2	39.81
2.218M	19	-2 5 2	40.65

d(Å)	I^{rel} σ = ±1	hkℓ	2θ(°)
2.218M		0 9 1	40.65
2.160M	7	0 10 0	41.78
2.160M		1 5 2	41.78
2.144	3	-3 5 1	42.12
2.137	4	-2 8 1	42.25
2.124	3	3 5 0	42.53
2.100	10	-2 6 2	43.03
2.091	10	-3 2 2	43.23
2.070M	9	1 10 0	43.69
2.070M		1 9 1	43.69
2.036	17	-3 6 1	44.47
2.007M	7	2 2 2	45.13
2.007M		2 9 0	45.13
1.994M	6	3 3 1	45.44
1.994M		-1 10 1	45.44
1.978	6	-2 9 1	45.85
1.951	3	-1 2 3	46.51
1.9111+	11	-1 3 3	47.54
1.9111+		-3 5 2	47.54
1.8961M	3	0 2 3	47.94
1.8961M		1 11 0	47.94
1.8784	3	-4 0 1	48.42
1.8604+	4	0 3 3	48.92
1.8604+		2 10 0	48.92
1.8466M	7	2 5 2	49.31
1.8466M		0 9 2	49.31
1.8371	18	-2 10 1	49.58
1.8098	10	3 8 0	50.38

CAS registry no.
10022-52-3

Sample
The sample was made by reaction between $SrCO_3$ and H_2BrO_3.

Color
Colorless

Structure
Monoclinic, $P2_1/n$ (14), Z = 4. The cell was obtained from axial ratios of Groth [1908], assuming Z = 4 and using a density of 3.778 as quoted by Groth [1908]. The space group was assumed from the peak absences.

Lattice constants of this sample

a = 9.375(2) Å
b = 7.6205(12)
c = 8.877(2)
β = 91.86(2)°

a/b = 1.2302
c/b = 1.1648

Volume
633.8 $Å^3$

Density
(calculated) 3.788 g/cm^3

Figure of merit
F_{30} = 35.3(0.012,74)

Reference intensity
$I/I_{corundum}$ = 2.7(2)

Reference
Groth, P. (1908). Chemische Krystallographie II, (Wilhelm Engelmann, Leipzig, Germany) p. 113.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
5.91	6	1 1 0	14.97
5.779	33	0 1 1	15.32
4.687	4	2 0 0	18.92
4.434	23	0 0 2	20.01
3.836	12	0 1 2	23.17
3.811	32	0 2 0	23.32
3.681	6	-2 1 1	24.16
3.586	31	-1 1 2	24.81
3.515	20	1 1 2	25.32
3.293	32	-1 2 1	27.06
3.275	39	-2 0 2	27.21
3.171	47	2 0 2	28.12
2.956	47	2 2 0	30.21
2.891M	100	0 2 2	30.91
2.891M		3 1 0	30.91
2.757	3	0 1 3	32.45
2.484	5	-2 2 2	36.13
2.453	13	1 3 0	36.60
2.445	13	0 3 1	36.72
2.438	11	2 2 2	36.83
2.409	2	-2 1 3	37.30
2.345+	5	2 1 3	38.36
2.345+		-3 2 1	38.36
2.316	16	3 2 1	38.85
2.281	4	-1 2 3	39.47
2.254	2	1 2 3	39.97
2.217	25	0 0 4	40.66
2.188	8	-4 1 1	41.23
2.173	4	-2 3 1	41.52
2.156M	8	4 1 1	41.86
2.156M		2 3 1	41.86
2.138	3	1 3 2	42.23
2.099M	6	-3 1 3	43.07
2.099M		3 2 2	43.07
2.063	1	1 1 4	43.85
2.044	2	4 0 2	44.27
1.9160+	4	2 1 4	47.41
1.9160+		0 2 4	47.41
1.8931	5	-3 2 3	48.02
1.8237	9	1 4 1	49.97
1.8189	11	5 1 0	50.11
1.8145	10	-3 3 2	50.24
1.7876	19	3 3 2	51.05
1.7651	10	2 4 0	51.75
1.7591	10	4 1 3	51.94
1.7509	11	0 4 2	52.20
1.7343+	7	3 1 4	52.74
1.7343+		-2 4 1	52.74
1.7020	9	-5 1 2	53.82
1.6832	1	4 3 1	54.47
1.6649	7	5 1 2	55.12
1.6514	2	-1 3 4	55.61
1.6341M	4	4 2 3	56.25
1.6341M		2 4 2	56.25
1.6043	2	-3 4 1	57.39
1.5921	3	4 3 2	57.87
1.5829	2	-1 4 3	58.24
1.5617M	2	2 3 4	59.11
1.5617M		6 0 0	59.11
1.5077+	7	2 2 5	61.45
1.5077+		5 3 0	61.45
1.4774	2	4 4 0	62.85

Strontium Chromium Oxide, $SrCr_2O_7$

Synonym
1. Strontium dichromate

Sample
The sample was prepared by heating $SrCr_2O_7 \cdot 3H_2O$ at 130 °C for 18 hours, followed by heating at 150 °C for 24 hours.

Color
Deep orange yellow

Structure
Tetragonal, $P4_2/nmc$ (137), Z = 8, isostructural with $PbCr_2O_7$. The structure of $SrCr_2O_7$ was determined by Wilhelmi [1967].

Lattice constants of this sample

a = 11.1925(7) Å
c = 9.4833(11)

c/a = 0.8473

Volume
1188.0 $Å^3$

Density
(calculated) 3.395 g/cm^3

Figure of merit
F_{30} = 72.4(0.010,41)

Reference intensity
$I/I_{corundum}$ = 2.35(8)

Additional pattern
1. PDF card 20-1191 [Wilhelmi, 1967]

Reference
Wilhelmi, K.-A. (1967). Ark. Kemi 26, 149.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} $\sigma = \pm 2$	hkℓ	2θ(°)
7.91	2	1 1 0	11.17
7.24	2	1 0 1	12.22
5.601	5	2 0 0	15.81
4.739	3	0 0 2	18.71
4.423	11	2 1 1	20.06
4.070	4	1 1 2	21.82
3.955	2	2 2 0	22.46
3.619	68	2 0 2	24.58
3.538	4	3 1 0	25.15
3.474	25	3 0 1	25.62
3.443	5	2 1 2	25.86
3.315	100	3 1 1	26.87
3.040M	32	1 0 3	29.36
3.040M		2 2 2	29.36
2.950	15	3 2 1	30.27
2.931	11	3 0 2	30.47
2.836	3	3 1 2	31.52
2.796	2	4 0 0	31.98
2.751	1	2 0 3	32.52
2.673	2	2 1 3	33.50
2.636	2	3 3 0	33.98
2.609	1	4 1 1	34.34
2.596	2	3 2 2	34.52
2.503	9	4 2 0	35.85
2.420	7	4 2 1	37.12
2.413	9	3 0 3	37.24
2.357M	11	3 1 3	38.15
2.357M		4 1 2	38.15
2.305	6	3 3 2	39.04
2.2145M	12	3 2 3	40.71
2.2145M		4 2 2	40.71
2.1944	7	5 1 0	41.10
2.1787	15	4 3 1	41.41
2.1388	3	5 1 1	42.22
2.0948	1	4 0 3	43.15
2.0304	29	5 2 1	44.59
2.0011	3	3 0 4	45.28
1.9779	2	4 4 0	45.84
1.9195	8	5 3 0	47.32
1.8835	1	3 2 4	48.28
1.8813	2	5 3 1	48.34
1.8654	8	6 0 0	48.78
1.8264M	13	4 3 3	49.89
1.8264M		4 4 2	49.89
1.8088	1	4 0 4	50.41

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
1.8038	2	5 1 3	50.56
1.7795	6	5 3 2	51.30
1.7635	5	3 3 4	51.80
1.7367M	2	5 2 3	52.66
1.7367M		6 0 2	52.66
1.7203	4	4 2 4	53.20
1.6909	4	3 0 5	54.20
1.6585	2	6 2 2	55.35
1.6432	1	6 3 1	55.91
1.6185	4	3 2 5	56.84
1.5904	1	6 1 3	57.94
1.5829	2	7 1 0	58.24
1.5770	2	7 0 1	58.48
1.5547	1	4 1 5	59.40
1.5502	1L	1 1 6	59.59
1.5316	1L	6 4 1	60.39
1.5175	3	7 2 1	61.01
1.5150	1L	7 0 2	61.12
1.5015	1	7 1 2	61.73
1.4699	2	7 3 0	63.21
1.4524	6	7 3 1	64.06

Strontium Chromium Oxide Hydrate, $SrCr_2O_7 \cdot 3H_2O$

Synonym
1. Strontium dichromate trihydrate

Sample
The sample was prepared by adding $SrCrO_4$ to a saturated solution of CrO_3. Large red crystals formed slowly.

Color
Unground, deep reddish brown. Ground, deep orange.

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The crystallographic information was obtained on a single crystal diffractometer by V. Himes. The cell parameters were confirmed by the Visser program [1969] and by axial ratios given by Groth [1908], assuming Z = 4 and a density near 2.6.

Lattice constants of this sample

a = 8.3583(12) Å
b = 14.023(2)
c = 7.574(2)
β = 91.95(2)°

a/b = 0.5960
c/b = 0.5401

Volume
887.22 $Å^3$

Density
(calculated) 2.678 g/cm^3

Figures of merit
F_{30} = 74.8 (0.010,40)
M_{20} = 38.4

Reference intensity
$I/I_{corundum}$ = 1.04(5)

References
Groth, P. (1908). Chemische Krystallographie II (Wilhelm Engelmann, Leipzig, Germany) p. 593.
Visser, J. W. (1969). J. Appl. Crystallogr. 2, 89.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±3	hkℓ	2θ(°)
8.35	31	1 0 0	10.59
7.18	9	1 1 0	12.31
7.02	8	0 2 0	12.60
6.67	4	0 1 1	13.27
5.368	9	1 2 0	16.50
5.286	25	-1 1 1	16.76
5.142M	10	0 2 1	17.23
5.142M		1 1 1	17.23
4.425	21	-1 2 1	20.05
4.337	20	1 2 1	20.46
4.178	100	2 0 0	21.25
4.079	23	1 3 0	21.77
4.001	68	2 1 0	22.20
3.980	70	0 3 1	22.32
3.784	45	0 0 2	23.49
3.652	25	0 1 2	24.35
3.614	25	-1 3 1	24.61
3.589M	10	2 2 0	24.79
3.589M		-2 1 1	24.79
3.504	45	0 4 0	25.40
3.388	21	-1 1 2	26.28
3.307	4	1 1 2	26.94
3.282	3	-2 2 1	27.15
3.230	17	1 4 0	27.59
3.208	35	2 2 1	27.79
3.181	7	0 4 1	28.03
3.128	4	-1 2 2	28.51
3.061	3	1 2 2	29.15
2.987	13	-1 4 1	29.89
2.958	14	1 4 1	30.19
2.907	13	-2 3 1	30.73
2.856M	15	2 3 1	31.29
2.856M		-2 0 2	31.29
2.785	20	3 0 0	32.11
2.752	7	1 3 2	32.51
2.731	6	3 1 0	32.76
2.706	20	2 1 2	33.08
2.686	9	2 4 0	33.33
2.657	10	1 5 0	33.70
2.597	15	-3 1 1	34.51
2.567	13	2 2 2	34.92
2.541	9	3 1 1	35.29
2.500	3	1 5 1	35.89
2.473M	7	-1 4 2	36.30
2.473M		-3 2 1	36.30

d(Å)	I^{rel} $\sigma = \pm 3$	hkℓ			2θ(°)
2.425	20	3	2	1	37.04
2.393	30	3	3	0	37.56
2.359	3	1	1	3	38.11
2.338	3	0	6	0	38.48
2.302M	9	-1	2	3	39.10
2.302M		-3	3	1	39.10
2.263M	1	1	2	3	39.80
2.263M		3	3	1	39.80
2.233	4	0	6	1	40.36
2.212M	5	2	5	1	40.75
2.212M		-2	4	2	40.75
2.186	4	-1	5	2	41.26
2.1662+	25	2	4	2	41.66
2.1662+		-2	1	3	41.66
2.1036M	16	3	2	2	42.96
2.1036M		2	1	3	42.96
2.0879	10	4	0	0	43.30
2.0648	2	4	1	0	43.81
2.0492M	13	-3	3	2	44.16
2.0492M		0	4	3	44.16
2.0103	12	-4	1	1	45.06
2.0028M	21	-1	4	3	45.24
2.0028M		4	2	0	45.24
1.9767M	32	1	4	3	45.87
1.9767M		3	5	0	45.87
1.9622	5	2	6	1	46.23
1.9376M	24	0	7	1	46.85
1.9376M		2	3	3	46.85

Synonym
1. Hydrazinecarbothioamide

CAS registry no.
79-19-6

Sample
The sample was obtained from J. T. Baker Co., Phillipsburg, NJ. It was recrystallized from ethanol.

Color
Colorless

Structure
Triclinic, $P\bar{1}$ (2), Z = 2. The structure was determined by Andreetti et al. [1970].

Lattice constants of this sample

a = 6.0266(12) Å
b = 7.327(2)
c = 4.9353(15)
α = 103.00(2)°
β = 96.33(2)
γ = 77.21(2)

a/b = 0.8225
c/b = 0.6736

Volume
206.65 $Å^3$

Density
(calculated) 1.465 g/cm^3

Figure of merit
F_{30} = 40.9(0.015,50)

Reference intensity
$I/I_{corundum}$ = 2.56(11)

Additional pattern
1. PDF card 24-1952 [Institute of Physics, University College, Cardiff, Wales]

Reference
Andreetti, G. D., Domiano, P., Gasparri, G. F., Nardelli, M., and Sgarabotto, P. (1970). Acta Crystallogr. B26, 1005.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
5.86	5	1 0 0	15.11
5.021	18	1 1 0	17.65
4.797	13	0 0 1	18.48
4.399	5	0 -1 1	20.17
4.100	4	-1 1 0	21.66
3.619	36	0 1 1	24.58
3.497	11	0 2 0	25.45
3.309	1	1 2 0	26.92
3.245	11	1 -1 1	27.46
3.163	100	1 1 1	28.19
3.082	7	-1 -2 1	28.95
3.008	8	-1 1 1	29.68
2.931	6	2 0 0	30.47
2.767	1L	-1 2 0	32.33
2.685	1	-2 -1 1	33.35
2.582	1	0 2 1	34.71
2.548	2	1 -2 1	35.19
2.527	4	-2 1 0	35.49
2.512	1	2 2 0	35.71
2.472	3	1 2 1	36.31
2.437M	2	-2 -2 1	36.86
2.437M		2 0 1	36.86
2.333	2	1 3 0	38.56
2.291	1L	0 -3 1	39.29
2.271M	1L	-1 0 2	39.66
2.271M		-1 2 1	39.66
2.202M	2	0 -2 2	40.95
2.202M		-1 -2 2	40.95
2.173	2	1 0 2	41.52
2.143	1	1 -1 2	42.13
2.138	1L	0 1 2	42.23
2.051	2	-2 2 0	44.13
2.037	1	2 3 0	44.44
2.008	2	-2 -1 2	45.11
1.990	1	3 1 0	45.54
1.985	2	1 -3 1	45.66
1.945M	1	1 -2 2	46.66
1.945M		0 3 1	46.66
1.929	1L	1 3 1	47.06
1.925	1L	-3 -1 1	47.18

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
1.877M	1L	0 -3 2	48.47
1.877M		3 2 0	48.47
1.859	2	-3 -2 1	48.95
1.836	1	-2 2 1	49.61
1.811	1	0 2 2	50.35
1.8025	1	2 0 2	50.60
1.7906	1	-3 1 0	50.96
1.7724M	2	3 0 1	51.52
1.7724M		-1 3 1	51.52
1.7594+	4	-2 -3 2	51.93
1.7594+		1 2 2	51.93
1.7315	2	2 1 2	52.83
1.7034	1L	-1 2 2	53.77
1.6907M	1L	-2 -4 1	54.21
1.6907M		-3 -3 1	54.21
1.6741M	1	3 -1 1	54.79
1.6741M		3 3 0	54.79
1.6541	1L	3 2 1	55.51
1.6219M	1	-1 -1 3	56.71
1.6219M		2 -2 2	56.71

Thiourea, CH_4N_2S

Synonym
1. Thiocarbamide

CAS registry no.
62-56-6

Sample
The sample was obtained from J. T. Baker Chemical Co., Phillipsburg, NJ. It was recrystallized from ethanol.

Color
Colorless

Structure
Orthorhombic, Pnma (62), Z = 4. The structure was first determined by Demeny and Nitta, [1928]. It was later refined by Truter [1957].

Lattice constants of this sample

a = 7.6644(12) Å
b = 8.5591(12)
c = 5.4925(8)

a/b = 0.8955
c/b = 0.6417

Volume
360.31 $Å^3$

Density
(calculated) 1.403 g/cm^3

Figure of merit
F_{30} = 66.3(0.009,49)

Reference intensity
$I/I_{corundum}$ = 0.91(3)

Additional pattern
1. PDF card 9-790 [Morse and Baun, Wright Patterson Air Force Base, Ohio]

References
Demeny, L. and Nitta, I. (1928). Bull. Chem. Soc. Japan 3, 128.
Truter, M. R. (1957). Acta Crystallogr. 10, 786.

$CuK\alpha_1$ λ = 1.540598 Å; temp. 25±1 °C

Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
4.624	9	0 1 1	19.18
4.467	70	1 0 1	19.86
4.279	100	0 2 0	20.74
3.834	61	2 0 0	23.18
3.498	53	2 1 0	25.44
3.142	65	2 0 1	28.38
3.089	66	1 2 1	28.88
2.951	24	2 1 1	30.26
2.855	45	2 2 0	31.31
2.747	8	0 0 2	32.57
2.532M	28	2 2 1	35.43
2.532M		0 3 1	35.43
2.475	31	1 1 2	36.26
2.405	1	1 3 1	37.36
2.317	9	3 0 1	38.83
2.2885	3	2 3 0	39.34
2.1598	7	2 1 2	41.79
2.1393	2	0 4 0	42.21
2.1116	5	2 3 1	42.79
2.0369	8	3 2 1	44.44
1.9291	14	1 4 1	47.07
1.9164M	5	4 0 0	47.40
1.9164M		1 3 2	47.40
1.8683	9	2 4 0	48.70
1.8271	8	3 1 2	49.87
1.7902	7	0 1 3	50.97
1.7695M	11	4 1 1	51.61
1.7695M		2 4 1	51.61
1.7487	3	4 2 0	52.27
1.7135	1	3 2 2	53.43
1.6883	1	0 4 2	54.29
1.6665	1L	4 2 1	55.06
1.6440	4	1 2 3	55.88
1.6346	2	0 5 1	56.23
1.6219	3	2 1 3	56.71
1.5716M	3	3 4 1	58.70
1.5716M		4 0 2	58.70
1.5643	4	3 3 2	59.00

Synonym
1. Stannous chloride dihydrate

CAS registry no.
10025-69-1

Sample
The sample was obtained from Fisher Scientific Co., Fair Lawn, NJ.

Color
Colorless

Structure
Monoclinic, $P2_1/c$ (14), Z = 4. The structure of $SnCl_2 \cdot 2H_2O$ was determined by Grdenic and Kamenar [1960].

Lattice constants of this sample

a = 9.318(3) Å
b = 7.2571(14)
c = 8.973(2)
β = 114.89(2)°

a/b = 1.2840
c/b = 1.2365

Volume
550.4 $Å^3$

Density
(calculated) 2.723 g/cm^3

Figure of merit
F_{30} = 49.4 (0.012,49)

Reference intensity
$I/I_{corundum}$ = 1.50(2)

Additional pattern
1. PDF card 20-1292 [University of Leeds, Leeds, England]

Reference
Grdenic, D. and Kamenar, B.(1960). Proc. Chem. Soc. 1960, 312.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C

Internal standard Si, a = 5.43088 Å

d(Å)	I^{rel} σ = ±8	hkℓ	2θ(°)
8.43	59	1 0 0	10.48
5.511	100	1 1 0	16.07
5.414	8	0 1 1	16.36
5.279	4	-1 1 1	16.78
4.483	1	-1 0 2	19.79
4.227	11	2 0 0	21.00
4.068M	19	1 1 1	21.83
4.068M		0 0 2	21.83
3.902	4	-2 1 1	22.77
3.810	53	-1 1 2	23.33
3.655	81	2 1 0	24.33
3.628	13	0 2 0	24.52
3.551	12	0 1 2	25.06
3.402	43	-2 1 2	26.17
3.334	8	1 2 0	26.72
3.181	8	1 0 2	28.03
2.953	6	2 1 1	30.24
2.912	5	1 1 2	30.68
2.819M	28	-1 2 2	31.72
2.819M		3 0 0	31.72
2.754M	20	-3 1 2	32.49
2.754M		2 2 0	32.49
2.709	60	0 2 2	33.04
2.642	34	-2 2 2	33.90
2.627	22	3 1 0	34.10
2.541	6	0 1 3	35.29
2.461	14	2 0 2	36.48
2.420	4	-3 1 3	37.12
2.392	19	1 2 2	37.57
2.327	24	1 3 0	38.67
2.318M	25	0 3 1	38.82
2.318M		-4 0 2	38.82
2.303	25	-3 2 2	39.09
2.253	2	3 1 1	39.99
2.238	10	-2 0 4	40.26
2.225	2	3 2 0	40.51
2.206M	2	-4 1 2	40.87
2.206M		1 1 3	40.87
2.171	3	1 3 1	41.57
2.138	7	-2 1 4	42.24
2.130M	20	-3 0 4	42.41
2.130M		-1 3 2	42.41
2.113	4	4 0 0	42.75
2.100	25	2 3 0	43.04
2.079	4	0 3 2	43.50
2.048	12	-2 3 2	44.18
2.035M	3	2 2 2	44.49
2.035M		0 0 4	44.49
1.960	10	0 1 4	46.29
1.953M	12	-4 2 2	46.47

d(Å)	I^{rel} $\sigma = \pm 8$	hkℓ	2θ(°)
1.953M		1 2 3	46.47
1.924M	4	-4 0 4	47.19
1.924M		1 3 2	47.19
1.905M	9	-3 3 1	47.71
1.905M		-2 2 4	47.71
1.894	10	3 1 2	47.99
1.8766M	4	-1 3 3	48.47
1.8766M		2 1 3	48.47
1.8618M	8	-4 1 4	48.88
1.8618M		-4 2 3	48.88
1.8357M	9	-3 2 4	49.62
1.8357M		3 3 0	49.62
1.8264	17	4 2 0	49.89
1.8142	17	0 4 0	50.25
1.8061M	14	0 3 3	50.49
1.8061M		-5 1 2	50.49
1.7734	8	1 4 0	51.49
1.7610M	6	-3 3 3	51.88
1.7610M		-5 1 1	51.88
1.7246	8	2 3 2	53.06

CAS registry no.
12039-90-6

Sample
The sample was prepared at NBS by R. F. Walker and S. Y. Holley. The sample had a small amount of ZrO_2 and Si present.

Major impurities
>1% Hf; 0.1 to 1.0 % Aℓ; 0.01 to 0.1% each Fe, Ni, and Ti; and 0.001 to 0.01% each Ca, Cr, and Mn.

Structure
Orthorhombic, Cmcm (63), Z = 4 [Seyfarth, 1928]. The structure was redetermined by Schachner et al. [1954] and by Vaughn and Bracuti [1958].

Lattice constants of this sample

a = 3.6958(3) Å
b = 14.7514(9)
c = 3.6654(3)

a/b = 0.2505
c/b = 0.2485

Volume
199.83 Å^3

Density
(calculated) 4.899 g/cm^3

Figure of merit
F_{30} = 81.8(0.009,40)

Additional pattern
1. PDF card 10-236 [Cotter et al., 1956].

References

Cotter, P. G., Kohn, J. A., and Potter, R. A. (1956). J. Amer. Ceram. Soc. 39, 11.
Schachner, H., Nowotny, H., and Kudielka, H. (1954). Monatsh. Chem. 85, 1140.
Seyfarth, H. (1928). Z. Kristallogr. Kristallgeometrie Kristallphys. Kristallchem. 67, 295.
Vaughn, P. A. and Bracuti, A. (1958). Diss. Abstr. B. 19, 1217.

CuKα_1 λ = 1.540598 Å; temp. 25±1 °C
Internal standard W, a = 3.16524 Å

d(Å)	I^{rel} σ = ±2	hkℓ	2θ(°)
7.37	4	0 2 0	12.00
3.685	9	0 4 0	24.13
3.586	15	1 1 0	24.81
3.283	32	0 2 1	27.14
2.954	15	1 3 0	30.23
2.601	1	0 4 1	34.46
2.564	10	1 1 1	34.97
2.458	15	0 6 0	36.53
2.300	100	1 3 1	39.14
2.0417	14	0 6 1	44.33
1.9518	1	1 5 1	46.49
1.8480	11	2 0 0	49.27
1.8434	7	0 8 0	49.40
1.8330	14	0 0 2	49.70
1.7782	1L	0 2 2	51.34
1.6519	2	2 4 0	55.59
1.6473	7	0 8 1	55.76
1.6381	7	1 7 1	56.10
1.6322	6	1 1 2	56.32
1.6102	7	2 2 1	57.16
1.5576	4	1 3 2	59.28
1.4982	6	1 9 0	61.88
1.4772	4	2 6 0	62.86
1.4692	5	0 6 2	63.24
1.4346	6	1 5 2	64.95
1.3867	2	1 9 1	67.49
1.3704	6	2 6 1	68.40
1.3050	1	2 8 0	72.35
1.3016	5	2 0 2	72.57
1.2603	1	1 11 0	75.35
1.2296M	3	2 8 1	77.58
1.2296M		0 12 0	77.58
1.2269	3	2 4 2	77.78
1.2051	1	0 2 3	79.46
1.1923	2	1 11 1	80.49
1.1655	1	0 12 1	82.74
1.1641	1	3 1 1	82.86
1.1602M	3	1 9 2	83.20
1.1602M		0 4 3	83.20
1.1502	2	2 6 2	84.09
1.1361	6	3 3 1	85.38
1.1291	4	1 3 3	86.04
1.0998	1L	2 10 1	88.92
1.0942	1L	0 6 3	89.50
1.0849	1L	1 13 0	90.47
1.0631	1	2 8 2	92.87
1.0538	1	0 14 0	93.94
1.0386	1	1 11 2	95.75

CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1-10 and MONOGRAPH 25, SECTIONS 1-17, inclusive.

INORGANIC NAMES

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m - Monograph 25.

A mineral name in ( ) indicates a synthetic sample.

*Natural mineral

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Section 17 - Data for 54 Substances

5. AUTHOR(S)

Marlene C. Morris, Howard F. McMurdie, Eloise H. Evans, Boris Paretzkin, Camden R. Hubbard and Simon J. Carmel

6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20234

JCPDS - International Centre for Diffraction Data, Swarthmore, PA 19081

7. Contract/Grant No.

8. Type of Report & Period Covered

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9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP)

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10. SUPPLEMENTARY NOTES

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11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

Standard x-ray diffraction patterns are presented for 54 substances. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indices determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated and the refractive indices were measured in some cases.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

Crystal structures; lattice constants; powder patterns; reference intensities; standard; x-ray diffraction.

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